



Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 03:22 PM UTC

PDB ID : 7QAB / pdb_00007qab
BMRB ID : 51091
Title : NMR Solution Structure of mussel adhesive protein Pvfp-5b
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Deposited on : 2021-11-16

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

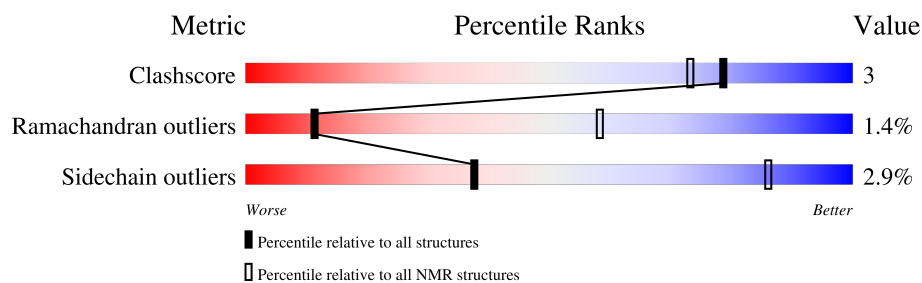
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	83	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:6-A:83 (78)	1.15	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 5, 7, 8, 10, 17, 18, 19, 20
2	4, 9, 16
3	12, 13, 15
4	6, 11
Single-model clusters	14

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1275 atoms, of which 612 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PVFP-5.

Mol	Chain	Residues	Atoms						Trace
1	A	83	Total	C	H	N	O	S	0
			1275	425	612	110	116	12	

There is a discrepancy between the modelled and reference sequences:

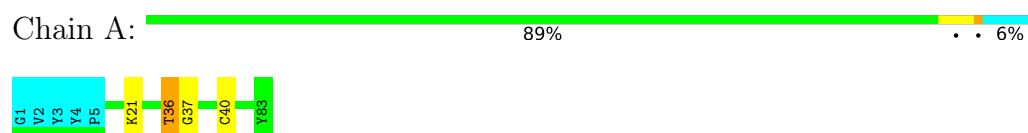
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP U5Y6P4

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: PVFP-5

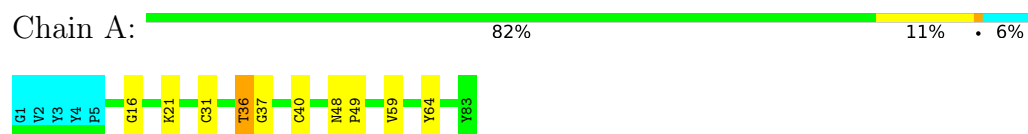


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

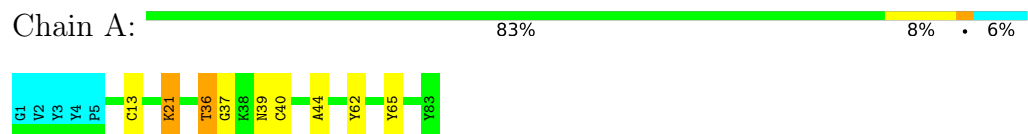
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: PVFP-5



4.2.2 Score per residue for model 2

- Molecule 1: PVFP-5



4.2.3 Score per residue for model 3

- Molecule 1: PVFP-5

Chain A:  82% 11% • 6%



4.2.4 Score per residue for model 4

- Molecule 1: PVFP-5

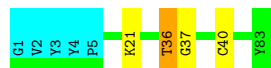
Chain A:  82% 12% 6%



4.2.5 Score per residue for model 5

- Molecule 1: PVFP-5

Chain A:  89% • • 6%



4.2.6 Score per residue for model 6

- Molecule 1: PVFP-5

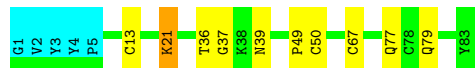
Chain A:  86% 7% • 6%



4.2.7 Score per residue for model 7

- Molecule 1: PVFP-5

Chain A:  82% 11% • 6%



4.2.8 Score per residue for model 8

- Molecule 1: PVFP-5

Chain A:  80% 14% 6%



4.2.9 Score per residue for model 9

- Molecule 1: PVFP-5

Chain A:  87% 6% 6%



4.2.10 Score per residue for model 10

- Molecule 1: PVFP-5

Chain A:  87% 7% 6%



4.2.11 Score per residue for model 11

- Molecule 1: PVFP-5

Chain A:  81% 13% 6%



4.2.12 Score per residue for model 12

- Molecule 1: PVFP-5

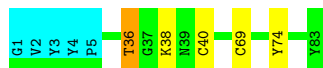
Chain A:  88% 6% 6%



4.2.13 Score per residue for model 13

- Molecule 1: PVFP-5

Chain A:  88% 5% • 6%



4.2.14 Score per residue for model 14

- Molecule 1: PVFP-5

Chain A:  87% 6% • 6%



4.2.15 Score per residue for model 15

- Molecule 1: PVFP-5

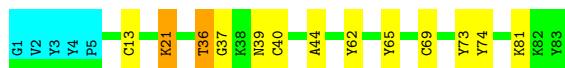
Chain A:  84% 7% • 6%



4.2.16 Score per residue for model 16

- Molecule 1: PVFP-5

Chain A:  78% 13% • 6%



4.2.17 Score per residue for model 17

- Molecule 1: PVFP-5

Chain A:  81% 13% • 6%



4.2.18 Score per residue for model 18

- Molecule 1: PVFP-5

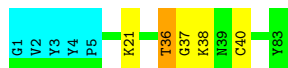
Chain A:  83% 10% • 6%



4.2.19 Score per residue for model 19

- Molecule 1: PVFP-5

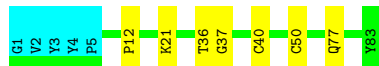
Chain A:  88% 5% • 6%



4.2.20 Score per residue for model 20

- Molecule 1: PVFP-5

Chain A:  86% 8% • 6%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	
ARIA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	944
Number of shifts mapped to atoms	944
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	621	573	573	3±2
All	All	12420	11460	11460	66

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:CYS:HA	1:A:39:ASN:O	0.64	1.92	7	7
1:A:36:THR:OG1	1:A:40:CYS:HA	0.61	1.96	16	11
1:A:62:TYR:HB2	1:A:65:TYR:O	0.59	1.96	14	5
1:A:13:CYS:HB3	1:A:40:CYS:SG	0.59	2.38	18	1
1:A:50:CYS:O	1:A:67:CYS:HB2	0.57	1.99	7	3
1:A:50:CYS:O	1:A:78:CYS:HB3	0.52	2.05	9	1
1:A:81:LYS:HB3	1:A:83:TYR:CE1	0.50	2.42	18	1
1:A:21:LYS:O	1:A:21:LYS:HD3	0.48	2.08	16	2
1:A:48:ASN:OD1	1:A:49:PRO:HD2	0.48	2.08	8	2
1:A:75:GLY:H	1:A:78:CYS:HA	0.47	1.67	11	3
1:A:7:PRO:O	1:A:27:TYR:HB3	0.47	2.08	18	1
1:A:21:LYS:HD3	1:A:21:LYS:H	0.47	1.68	19	3
1:A:69:CYS:SG	1:A:74:TYR:HA	0.47	2.49	8	3
1:A:48:ASN:HB3	1:A:50:CYS:SG	0.47	2.49	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:TYR:O	1:A:80:LEU:HB2	0.47	2.10	4	1
1:A:49:PRO:O	1:A:77:GLN:HB3	0.45	2.11	3	2
1:A:77:GLN:HB2	1:A:79:GLN:NE2	0.45	2.26	7	1
1:A:16:GLY:O	1:A:31:CYS:HA	0.44	2.13	1	2
1:A:50:CYS:O	1:A:78:CYS:HB2	0.44	2.13	18	1
1:A:44:ALA:HB1	1:A:65:TYR:HB3	0.44	1.88	16	2
1:A:11:TYR:CD1	1:A:29:CYS:HB2	0.43	2.48	11	1
1:A:17:GLY:HA2	1:A:30:TYR:O	0.43	2.13	11	1
1:A:82:LYS:C	1:A:82:LYS:HD3	0.42	2.38	8	3
1:A:50:CYS:HA	1:A:77:GLN:O	0.42	2.14	20	1
1:A:73:TYR:CD2	1:A:81:LYS:HA	0.42	2.50	16	1
1:A:82:LYS:HD2	1:A:83:TYR:N	0.41	2.31	3	1
1:A:22:ARG:C	1:A:24:LEU:H	0.41	2.23	8	2
1:A:15:ASN:O	1:A:32:ARG:HG2	0.40	2.16	17	1
1:A:63:PRO:HD2	1:A:65:TYR:CE2	0.40	2.51	6	1
1:A:59:VAL:O	1:A:64:TYR:HA	0.40	2.16	1	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	77/83 (93%)	67±1 (87±2%)	9±1 (12±2%)	1±0 (1±1%)	11	58
All	All	1540/1660 (93%)	1335 (87%)	184 (12%)	21 (1%)	11	58

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	37	GLY	17
1	A	63	PRO	3
1	A	12	PRO	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	66/70 (94%)	64±1 (97±1%)	2±1 (3±1%)	38	86
All	All	1320/1400 (94%)	1282 (97%)	38 (3%)	38	86

All 6 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	36	THR	20
1	A	21	LYS	13
1	A	38	LYS	2
1	A	13	CYS	1
1	A	33	LYS	1
1	A	40	CYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	944
Number of shifts mapped to atoms	944
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	82	0.40 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	70	0.01 ± 0.26	None needed (< 0.5 ppm)
$^{13}\text{C}'$	74	0.43 ± 0.21	None needed (< 0.5 ppm)
^{15}N	73	0.18 ± 0.55	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 884 atoms were assigned a chemical shift out of a possible 1002. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	375/387 (97%)	158/160 (99%)	147/156 (94%)	70/71 (99%)
Sidechain	379/470 (81%)	255/300 (85%)	124/143 (87%)	0/27 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	130/145 (90%)	65/65 (100%)	65/80 (81%)	0/0 (—%)
Overall	884/1002 (88%)	478/525 (91%)	336/379 (89%)	70/98 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 944 atoms were assigned a chemical shift out of a possible 1069. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	394/411 (96%)	165/170 (97%)	156/166 (94%)	73/75 (97%)
Sidechain	404/495 (82%)	272/317 (86%)	132/151 (87%)	0/27 (0%)
Aromatic	146/163 (90%)	73/73 (100%)	73/90 (81%)	0/0 (—%)
Overall	944/1069 (88%)	510/560 (91%)	361/407 (89%)	73/102 (72%)

7.1.4 Statistically unusual chemical shifts [i](#)

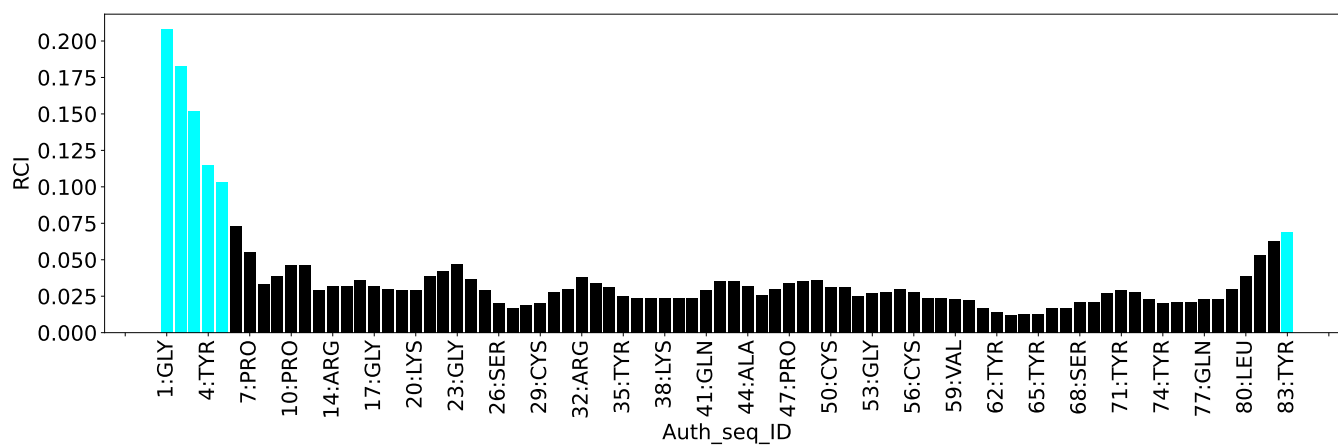
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	63	PRO	HA	2.75	2.78 – 6.00	-5.1

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1917
Intra-residue ($ i-j =0$)	735
Sequential ($ i-j =1$)	630
Medium range ($ i-j >1$ and $ i-j <5$)	164
Long range ($ i-j \geq 5$)	370
Inter-chain	0
Hydrogen bond restraints	18
Disulfide bond restraints	0
Total dihedral-angle restraints	112
Number of unmapped restraints	0
Number of restraints per residue	24.4
Number of long range restraints per residue ¹	4.7

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	68.5	0.2
0.2-0.5 (Medium)	178.6	0.5
>0.5 (Large)	391.4	4.75

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	10.3	8.63
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

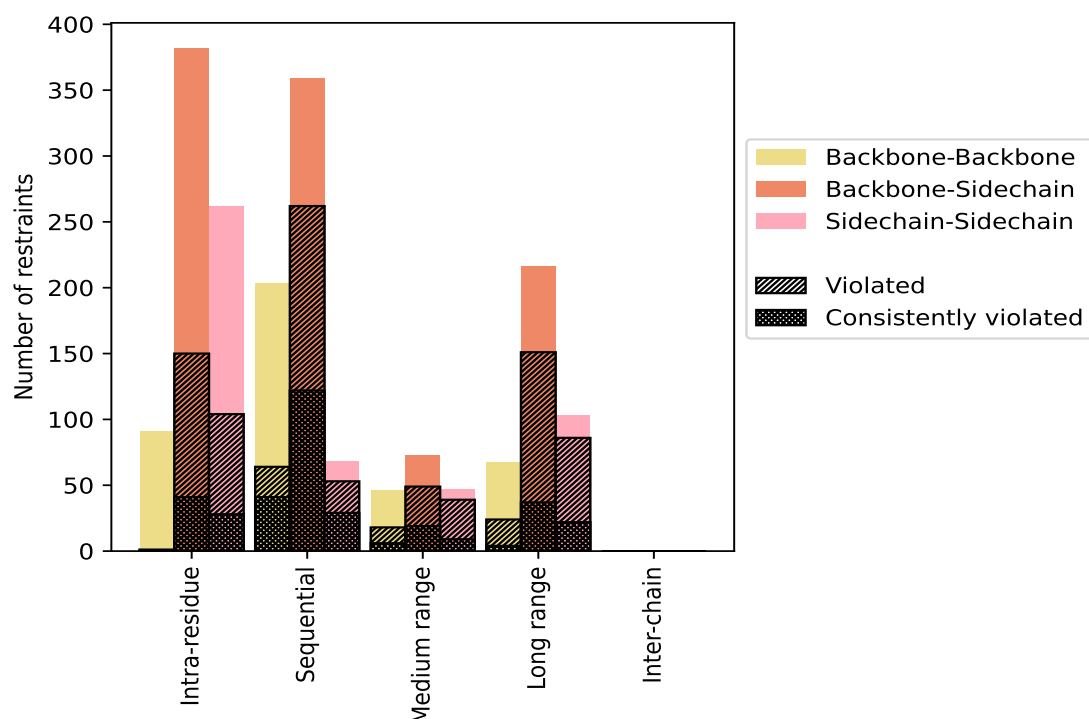
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	735	38.3	255	34.7	13.3	70	9.5	3.7
Backbone-Backbone	91	4.7	1	1.1	0.1	1	1.1	0.1
Backbone-Sidechain	382	19.9	150	39.3	7.8	41	10.7	2.1
Sidechain-Sidechain	262	13.7	104	39.7	5.4	28	10.7	1.5
Sequential ($i-j =1$)	630	32.9	379	60.2	19.8	192	30.5	10.0
Backbone-Backbone	203	10.6	64	31.5	3.3	41	20.2	2.1
Backbone-Sidechain	359	18.7	262	73.0	13.7	122	34.0	6.4
Sidechain-Sidechain	68	3.5	53	77.9	2.8	29	42.6	1.5
Medium range ($i-j >1$ & $i-j <5$)	164	8.6	106	64.6	5.5	34	20.7	1.8
Backbone-Backbone	46	2.4	18	39.1	0.9	6	13.0	0.3
Backbone-Sidechain	71	3.7	49	69.0	2.6	19	26.8	1.0
Sidechain-Sidechain	47	2.5	39	83.0	2.0	9	19.1	0.5
Long range ($i-j \geq 5$)	370	19.3	257	69.5	13.4	63	17.0	3.3
Backbone-Backbone	67	3.5	24	35.8	1.3	4	6.0	0.2
Backbone-Sidechain	200	10.4	147	73.5	7.7	37	18.5	1.9
Sidechain-Sidechain	103	5.4	86	83.5	4.5	22	21.4	1.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	18	0.9	4	22.2	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1917	100.0	1001	52.2	52.2	359	18.7	18.7
Backbone-Backbone	407	21.2	107	26.3	5.6	52	12.8	2.7
Backbone-Sidechain	1030	53.7	612	59.4	31.9	219	21.3	11.4
Sidechain-Sidechain	480	25.0	282	58.8	14.7	88	18.3	4.6

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	157	284	62	145	0	648	0.76	4.33	0.55	0.63
2	156	283	62	132	0	633	0.76	4.36	0.58	0.61
3	160	269	59	161	0	649	0.77	4.35	0.56	0.63
4	160	277	58	142	0	637	0.76	4.1	0.57	0.63
5	151	273	59	145	0	628	0.76	4.75	0.59	0.63
6	160	268	65	153	0	646	0.75	4.1	0.55	0.62
7	161	277	59	145	0	642	0.75	3.34	0.55	0.63
8	153	285	57	139	0	634	0.79	4.05	0.6	0.65
9	159	284	65	154	0	662	0.78	4.08	0.56	0.64
10	152	279	58	140	0	629	0.78	4.5	0.58	0.66

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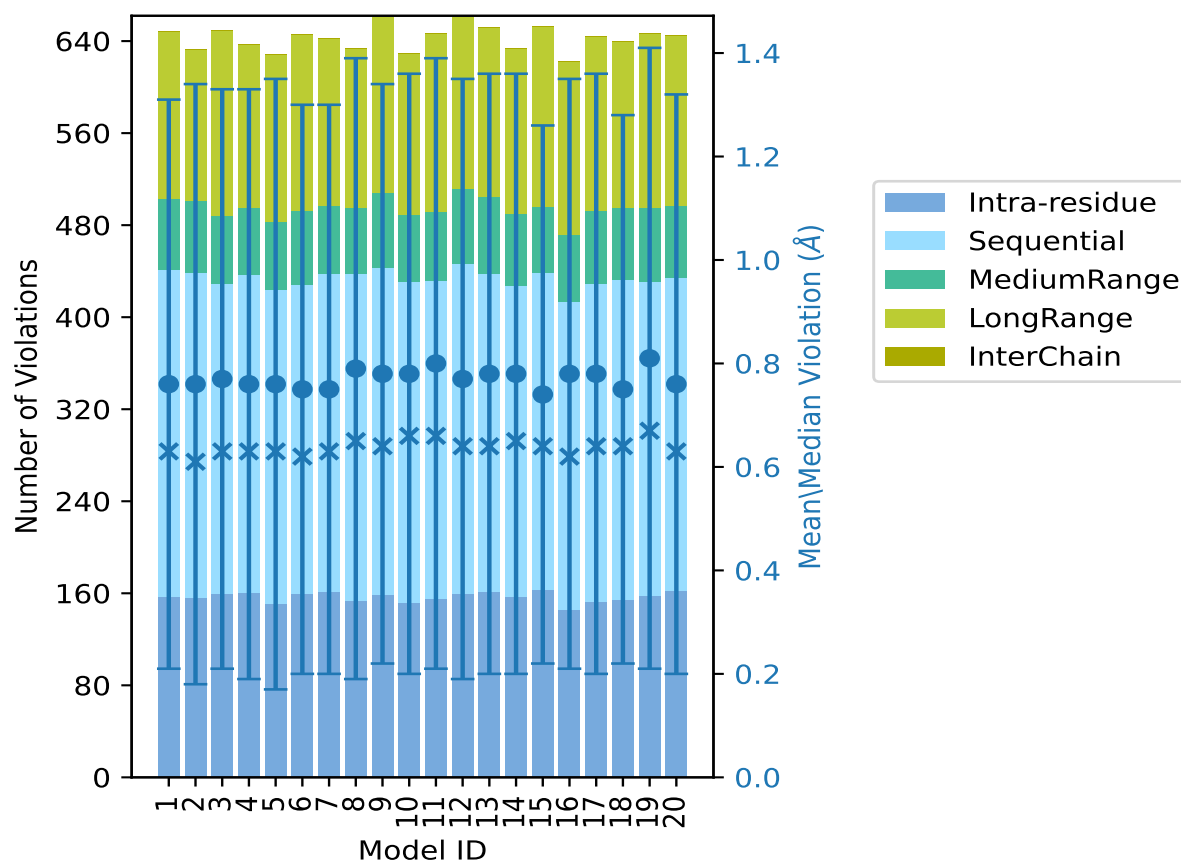
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	155	277	60	155	0	647	0.8	4.08	0.59	0.66
12	160	286	66	150	0	662	0.77	4.54	0.58	0.64
13	161	277	67	147	0	652	0.78	3.59	0.58	0.64
14	157	270	63	144	0	634	0.78	3.29	0.58	0.65
15	163	276	57	157	0	653	0.74	2.98	0.52	0.64
16	146	267	59	150	0	622	0.78	3.38	0.57	0.62
17	153	276	63	152	0	644	0.78	3.37	0.58	0.64
18	154	279	62	145	0	640	0.75	3.28	0.53	0.64
19	158	273	64	152	0	647	0.81	4.31	0.6	0.67
20	162	272	63	148	0	645	0.76	3.35	0.56	0.63

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble

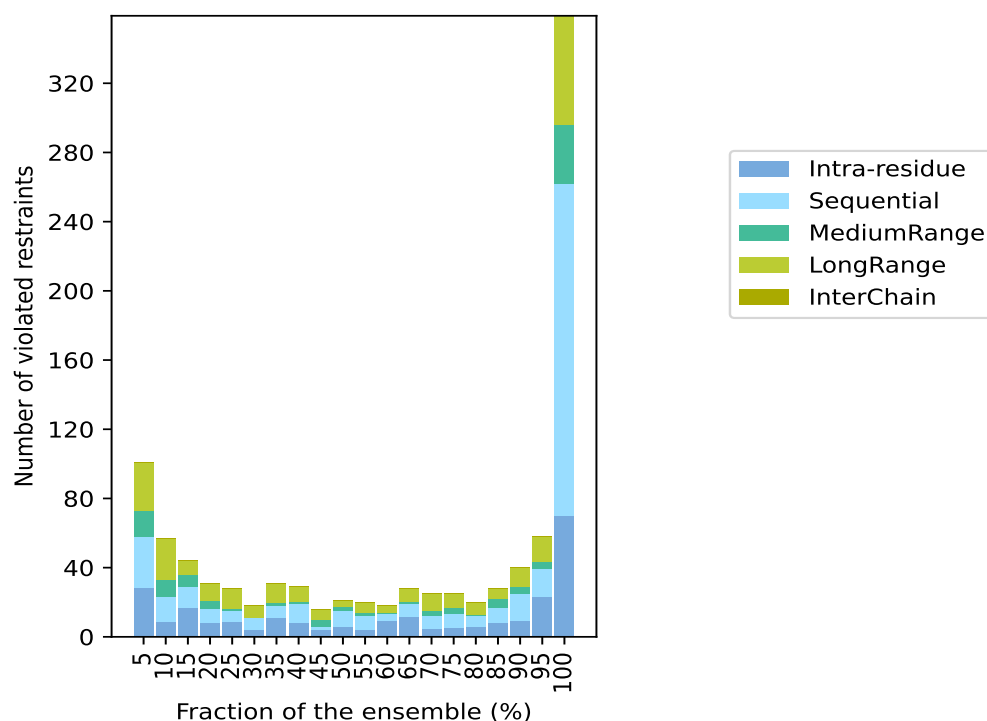
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 902(IR:480, SQ:251, MR:58, LR:113, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
28	30	15	28	0	101	1	5.0
9	14	10	24	0	57	2	10.0
17	12	7	8	0	44	3	15.0
8	8	5	10	0	31	4	20.0
9	6	1	12	0	28	5	25.0
4	7	0	7	0	18	6	30.0
11	7	2	11	0	31	7	35.0
8	11	1	9	0	29	8	40.0
4	2	4	6	0	16	9	45.0
6	9	2	4	0	21	10	50.0
4	8	2	6	0	20	11	55.0
9	4	1	4	0	18	12	60.0
12	7	1	8	0	28	13	65.0
5	7	3	10	0	25	14	70.0
5	8	4	8	0	25	15	75.0
6	6	1	7	0	20	16	80.0
8	9	5	6	0	28	17	85.0
9	16	4	11	0	40	18	90.0
23	16	4	15	0	58	19	95.0
70	192	34	63	0	359	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

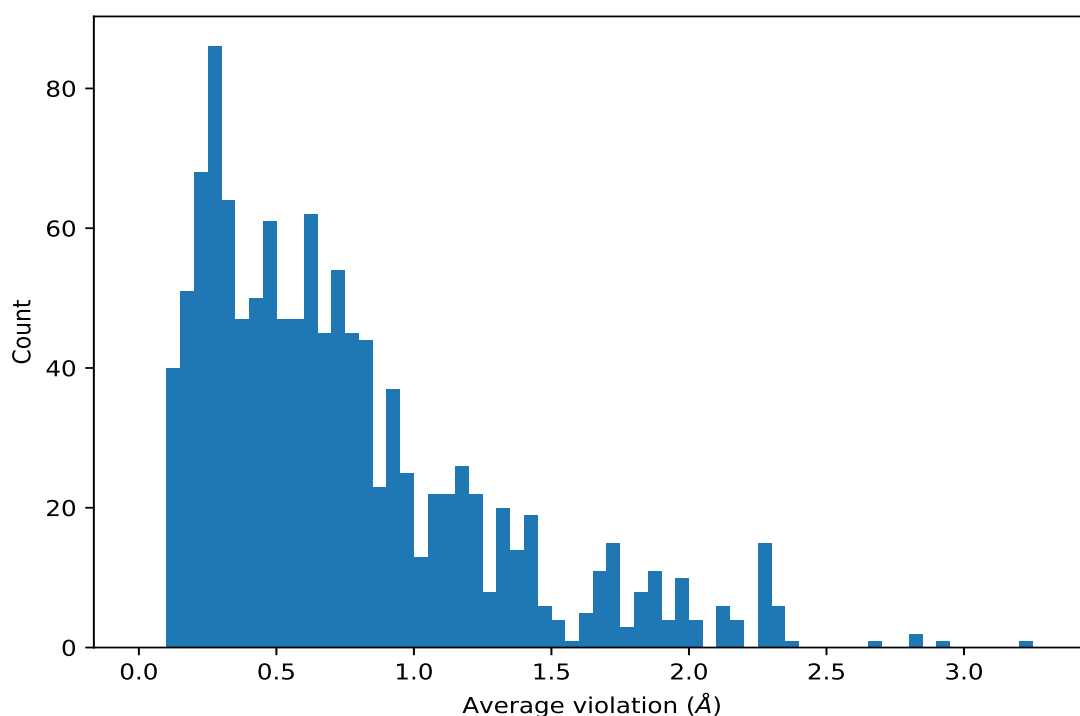
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	20	3.24	0.52	3.12
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	20	2.91	0.18	2.88
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	20	2.82	0.67	2.87
(1,26)	1:79:A:GLN:HB2	1:49:A:PRO:HA	20	2.82	0.67	2.87
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	20	2.66	0.62	2.8
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG11	20	2.3	0.25	2.27
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG13	20	2.3	0.25	2.27
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG12	20	2.3	0.25	2.27
(1,1028)	1:59:A:VAL:HG11	1:64:A:TYR:HB3	20	2.26	0.5	2.22
(1,1028)	1:59:A:VAL:HG13	1:64:A:TYR:HB3	20	2.26	0.5	2.22
(1,1028)	1:59:A:VAL:HG12	1:64:A:TYR:HB3	20	2.26	0.5	2.22
(1,694)	1:44:A:ALA:HB2	1:59:A:VAL:HG11	20	2.25	0.36	2.29
(1,694)	1:44:A:ALA:HB3	1:59:A:VAL:HG11	20	2.25	0.36	2.29
(1,694)	1:44:A:ALA:HB2	1:59:A:VAL:HG13	20	2.25	0.36	2.29
(1,694)	1:44:A:ALA:HB1	1:59:A:VAL:HG13	20	2.25	0.36	2.29
(1,694)	1:44:A:ALA:HB3	1:59:A:VAL:HG12	20	2.25	0.36	2.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,694)	1:44:A:ALA:HB1	1:59:A:VAL:HG12	20	2.25	0.36	2.29
(1,694)	1:44:A:ALA:HB3	1:59:A:VAL:HG13	20	2.25	0.36	2.29
(1,694)	1:44:A:ALA:HB2	1:59:A:VAL:HG12	20	2.25	0.36	2.29
(1,694)	1:44:A:ALA:HB1	1:59:A:VAL:HG11	20	2.25	0.36	2.29
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	20	2.17	0.02	2.17
(1,1027)	1:59:A:VAL:HG11	1:64:A:TYR:HB2	20	2.15	0.47	2.09
(1,1027)	1:59:A:VAL:HG13	1:64:A:TYR:HB2	20	2.15	0.47	2.09
(1,1027)	1:59:A:VAL:HG12	1:64:A:TYR:HB2	20	2.15	0.47	2.09
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	20	2.12	0.29	2.08
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD23	20	2.12	0.09	2.12
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	20	2.12	0.09	2.12
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD22	20	2.12	0.09	2.12
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	20	2.11	0.2	2.12
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	20	2.01	0.02	2.01
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG21	20	2.01	0.05	2.01
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG22	20	2.01	0.05	2.01
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG23	20	2.01	0.05	2.01
(1,867)	1:55:A:THR:HG23	1:54:A:GLY:HA2	20	1.98	0.08	2.0
(1,867)	1:55:A:THR:HG22	1:54:A:GLY:HA2	20	1.98	0.08	2.0
(1,867)	1:55:A:THR:HG21	1:54:A:GLY:HA2	20	1.98	0.08	2.0
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	20	1.96	0.48	2.07
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD21	20	1.95	0.02	1.95
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD22	20	1.95	0.02	1.95
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD23	20	1.95	0.02	1.95
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	20	1.93	0.12	1.96
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD23	20	1.9	0.14	1.88
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	20	1.9	0.14	1.88
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD22	20	1.9	0.14	1.88
(1,962)	1:59:A:VAL:HG22	1:65:A:TYR:H	20	1.87	0.31	1.94
(1,962)	1:59:A:VAL:HG23	1:65:A:TYR:H	20	1.87	0.31	1.94
(1,962)	1:59:A:VAL:HG21	1:65:A:TYR:H	20	1.87	0.31	1.94
(1,18)	1:59:A:VAL:HG13	1:63:A:PRO:HD2	20	1.86	0.23	1.86
(1,18)	1:59:A:VAL:HG13	1:60:A:TYR:HB2	20	1.86	0.23	1.86
(1,18)	1:59:A:VAL:HG12	1:60:A:TYR:HB2	20	1.86	0.23	1.86
(1,18)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	20	1.86	0.23	1.86
(1,18)	1:59:A:VAL:HG11	1:60:A:TYR:HB2	20	1.86	0.23	1.86
(1,18)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	20	1.86	0.23	1.86
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	20	1.85	0.24	1.83
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG22	20	1.84	0.3	1.79
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG23	20	1.84	0.3	1.79
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG21	20	1.84	0.3	1.79
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG22	20	1.83	1.52	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG21	20	1.83	1.52	0.9
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG23	20	1.83	1.52	0.9
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	20	1.82	0.29	1.69
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	20	1.8	0.1	1.81
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	20	1.79	0.07	1.78
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	20	1.77	0.48	1.74
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	20	1.76	0.23	1.82
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG21	20	1.74	0.11	1.74
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG22	20	1.74	0.11	1.74
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG23	20	1.74	0.11	1.74
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD13	20	1.74	0.06	1.74
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD11	20	1.74	0.06	1.74
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD12	20	1.74	0.06	1.74
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	20	1.74	0.63	2.0
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	20	1.71	0.04	1.7
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	20	1.7	0.34	1.73
(1,4)	1:7:A:PRO:HA	1:21:A:LYS:HE2	20	1.7	0.34	1.73
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG13	20	1.68	0.44	1.54
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG12	20	1.68	0.44	1.54
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG11	20	1.68	0.44	1.54
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	20	1.68	0.02	1.67
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG22	20	1.67	0.31	1.65
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG23	20	1.67	0.31	1.65
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG21	20	1.67	0.31	1.65
(1,948)	1:59:A:VAL:HG11	1:64:A:TYR:HA	20	1.65	0.56	1.6
(1,948)	1:59:A:VAL:HG13	1:64:A:TYR:HA	20	1.65	0.56	1.6
(1,948)	1:59:A:VAL:HG12	1:64:A:TYR:HA	20	1.65	0.56	1.6
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	20	1.63	0.16	1.61
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	20	1.62	0.36	1.52
(1,1005)	1:59:A:VAL:HG13	1:63:A:PRO:HD2	20	1.6	0.49	1.46
(1,1005)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	20	1.6	0.49	1.46
(1,1005)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	20	1.6	0.49	1.46
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	20	1.59	0.04	1.6
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	20	1.52	0.57	1.57
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	20	1.51	0.23	1.55
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	20	1.49	0.09	1.49
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	20	1.49	0.31	1.48
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	20	1.48	0.02	1.48
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	20	1.45	0.73	1.5
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	20	1.45	0.4	1.5
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	20	1.45	0.04	1.44
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	20	1.44	0.38	1.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	20	1.43	0.13	1.45
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	20	1.42	0.29	1.34
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	20	1.42	0.31	1.42
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	20	1.41	0.39	1.42
(1,790)	1:51:A:LEU:HD12	1:51:A:LEU:HA	20	1.41	0.02	1.41
(1,790)	1:51:A:LEU:HD13	1:51:A:LEU:HA	20	1.41	0.02	1.41
(1,790)	1:51:A:LEU:HD11	1:51:A:LEU:HA	20	1.41	0.02	1.41
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	20	1.4	0.51	1.52
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	20	1.4	0.03	1.4
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	20	1.4	0.18	1.31
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	20	1.38	0.09	1.39
(1,943)	1:59:A:VAL:HG11	1:65:A:TYR:HB3	20	1.38	0.32	1.42
(1,943)	1:59:A:VAL:HG13	1:65:A:TYR:HB3	20	1.38	0.32	1.42
(1,943)	1:59:A:VAL:HG12	1:65:A:TYR:HB3	20	1.38	0.32	1.42
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	20	1.37	0.04	1.38
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD12	20	1.37	0.04	1.38
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD13	20	1.37	0.04	1.38
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	20	1.37	0.26	1.27
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	20	1.37	0.29	1.33
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	20	1.36	0.05	1.36
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	20	1.35	0.02	1.35
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	20	1.35	0.53	1.48
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	20	1.35	0.52	1.2
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	20	1.35	0.72	1.17
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	20	1.34	0.47	1.27
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	20	1.34	0.35	1.33
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	20	1.33	0.29	1.33
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	20	1.33	0.17	1.33
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	20	1.33	0.35	1.27
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	20	1.33	0.05	1.33
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	20	1.32	0.1	1.32
(1,952)	1:59:A:VAL:HG11	1:58:A:TYR:HD1	20	1.32	0.33	1.25
(1,952)	1:59:A:VAL:HG13	1:58:A:TYR:HD1	20	1.32	0.33	1.25
(1,952)	1:59:A:VAL:HG12	1:58:A:TYR:HD1	20	1.32	0.33	1.25
(1,965)	1:59:A:VAL:HG22	1:64:A:TYR:H	20	1.3	0.41	1.34
(1,965)	1:59:A:VAL:HG23	1:64:A:TYR:H	20	1.3	0.41	1.34
(1,965)	1:59:A:VAL:HG21	1:64:A:TYR:H	20	1.3	0.41	1.34
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	20	1.3	0.07	1.28
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	20	1.3	0.25	1.23
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	20	1.3	0.15	1.34
(1,306)	1:18:A:THR:HG21	1:20:A:LYS:HA	20	1.3	0.13	1.28
(1,306)	1:18:A:THR:HG22	1:20:A:LYS:HA	20	1.3	0.13	1.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,306)	1:18:A:THR:HG23	1:20:A:LYS:HA	20	1.3	0.13	1.28
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	20	1.28	0.11	1.28
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	20	1.28	0.3	1.27
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	20	1.27	0.27	1.23
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	20	1.27	0.1	1.28
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	20	1.25	0.04	1.25
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	20	1.24	0.07	1.24
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	20	1.23	0.17	1.27
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	20	1.23	0.22	1.17
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	20	1.23	0.1	1.21
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	20	1.22	0.26	1.16
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	20	1.22	0.61	1.28
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	20	1.22	0.09	1.19
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	20	1.21	0.09	1.19
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	20	1.2	0.64	1.1
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	20	1.2	0.08	1.23
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	20	1.2	0.06	1.19
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG23	20	1.2	0.26	1.23
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG21	20	1.2	0.26	1.23
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG22	20	1.2	0.26	1.23
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG22	20	1.19	0.04	1.19
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG23	20	1.19	0.04	1.19
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG21	20	1.19	0.04	1.19
(1,706)	1:44:A:ALA:HB1	1:64:A:TYR:HD1	20	1.19	0.28	1.12
(1,706)	1:44:A:ALA:HB2	1:64:A:TYR:HD1	20	1.19	0.28	1.12
(1,706)	1:44:A:ALA:HB3	1:64:A:TYR:HD1	20	1.19	0.28	1.12
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	20	1.19	0.2	1.23
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	20	1.19	0.24	1.18
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	20	1.19	0.18	1.16
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD12	20	1.19	0.18	1.16
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD13	20	1.19	0.18	1.16
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	20	1.17	0.92	0.85
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	20	1.16	0.17	1.12
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	20	1.16	0.22	1.11
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	20	1.16	0.17	1.16
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	20	1.16	0.09	1.16
(1,953)	1:59:A:VAL:HG13	1:60:A:TYR:HD1	20	1.16	0.33	1.24
(1,953)	1:59:A:VAL:HG12	1:60:A:TYR:HD1	20	1.16	0.33	1.24
(1,953)	1:59:A:VAL:HG11	1:60:A:TYR:HD1	20	1.16	0.33	1.24
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	20	1.15	0.5	0.82
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	20	1.15	0.08	1.13
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	20	1.15	0.75	1.03

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	20	1.14	0.24	1.19
(1,869)	1:55:A:THR:HG22	1:68:A:SER:HB3	20	1.14	0.32	1.19
(1,869)	1:55:A:THR:HG21	1:68:A:SER:HB3	20	1.14	0.32	1.19
(1,869)	1:55:A:THR:HG23	1:68:A:SER:HB3	20	1.14	0.32	1.19
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	20	1.14	0.22	1.1
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	20	1.13	0.49	1.04
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	20	1.13	0.18	1.1
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	20	1.13	0.22	1.1
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	20	1.13	0.33	1.06
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	20	1.12	0.11	1.11
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	20	1.11	0.09	1.12
(1,866)	1:55:A:THR:HG21	1:56:A:CYS:HB2	20	1.1	0.09	1.12
(1,866)	1:55:A:THR:HG23	1:56:A:CYS:HB2	20	1.1	0.09	1.12
(1,866)	1:55:A:THR:HG22	1:56:A:CYS:HB2	20	1.1	0.09	1.12
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	20	1.09	0.34	1.02
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	20	1.09	0.03	1.1
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	20	1.08	0.31	1.03
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	20	1.07	0.02	1.07
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	20	1.07	0.07	1.08
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	20	1.06	0.44	1.08
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG11	20	1.06	0.34	1.02
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG13	20	1.06	0.34	1.02
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG12	20	1.06	0.34	1.02
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	20	1.05	0.2	1.13
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	20	1.05	0.23	1.09
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	20	1.05	0.44	0.83
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	20	1.04	0.4	1.08
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	20	1.04	0.25	1.1
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	20	1.03	0.17	1.05
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG23	20	1.0	0.21	1.04
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG21	20	1.0	0.21	1.04
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG22	20	1.0	0.21	1.04
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	20	1.0	0.02	0.99
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD21	20	0.99	0.1	1.0
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	20	0.99	0.1	1.0
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD23	20	0.99	0.1	1.0
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	20	0.99	0.18	1.0
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	20	0.99	0.36	1.23
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	20	0.99	0.1	0.96
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	20	0.98	0.11	0.94
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	20	0.98	0.12	0.98
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	20	0.97	0.1	0.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	20	0.96	0.14	0.93
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	20	0.95	0.13	0.9
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD13	20	0.95	0.13	0.9
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD11	20	0.95	0.13	0.9
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	20	0.95	0.06	0.94
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD23	20	0.94	0.12	0.94
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	20	0.94	0.12	0.94
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD22	20	0.94	0.12	0.94
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	20	0.94	0.26	0.86
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	20	0.94	0.66	1.02
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	20	0.93	0.22	0.92
(1,305)	1:18:A:THR:HG21	1:17:A:GLY:HA2	20	0.93	0.05	0.94
(1,305)	1:18:A:THR:HG23	1:17:A:GLY:HA2	20	0.93	0.05	0.94
(1,305)	1:18:A:THR:HG22	1:17:A:GLY:HA2	20	0.93	0.05	0.94
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD22	20	0.93	0.01	0.94
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD23	20	0.93	0.01	0.94
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD21	20	0.93	0.01	0.94
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	20	0.93	0.25	1.01
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	20	0.92	0.19	0.9
(1,873)	1:55:A:THR:H	1:55:A:THR:HG21	20	0.92	0.03	0.92
(1,873)	1:55:A:THR:H	1:55:A:THR:HG23	20	0.92	0.03	0.92
(1,873)	1:55:A:THR:H	1:55:A:THR:HG22	20	0.92	0.03	0.92
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	20	0.92	0.08	0.93
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	20	0.91	0.29	0.8
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	20	0.91	0.29	0.96
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	20	0.91	0.03	0.92
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB1	20	0.91	0.1	0.91
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB2	20	0.91	0.1	0.91
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB3	20	0.91	0.1	0.91
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD23	20	0.91	0.17	0.94
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	20	0.91	0.17	0.94
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD22	20	0.91	0.17	0.94
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	20	0.91	0.01	0.91
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	20	0.89	0.01	0.89
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	20	0.89	0.43	0.81
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	20	0.88	0.05	0.88
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	20	0.87	0.21	0.89
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	20	0.87	0.24	0.9
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	20	0.87	0.2	0.78
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	20	0.86	0.01	0.86
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	20	0.85	0.06	0.86
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	20	0.85	0.28	0.78

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	20	0.83	0.05	0.83
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	20	0.82	0.03	0.82
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	20	0.82	0.05	0.84
(1,1316)	1:80:A:LEU:HD21	1:80:A:LEU:HB2	20	0.82	0.01	0.82
(1,1316)	1:80:A:LEU:HD22	1:80:A:LEU:HB2	20	0.82	0.01	0.82
(1,1316)	1:80:A:LEU:HD23	1:80:A:LEU:HB2	20	0.82	0.01	0.82
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	20	0.82	0.05	0.81
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	20	0.82	0.09	0.82
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	20	0.81	0.15	0.86
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	20	0.81	0.11	0.84
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD13	20	0.81	0.11	0.84
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD11	20	0.81	0.11	0.84
(1,865)	1:55:A:THR:HG21	1:56:A:CYS:HB3	20	0.81	0.17	0.8
(1,865)	1:55:A:THR:HG23	1:56:A:CYS:HB3	20	0.81	0.17	0.8
(1,865)	1:55:A:THR:HG22	1:56:A:CYS:HB3	20	0.81	0.17	0.8
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	20	0.81	0.33	0.68
(1,703)	1:44:A:ALA:HB3	1:58:A:TYR:HA	20	0.81	0.29	0.81
(1,703)	1:44:A:ALA:HB1	1:58:A:TYR:HA	20	0.81	0.29	0.81
(1,703)	1:44:A:ALA:HB2	1:58:A:TYR:HA	20	0.81	0.29	0.81
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	20	0.81	0.35	0.76
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	20	0.8	0.7	0.54
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	20	0.8	0.05	0.8
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	20	0.8	0.09	0.79
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	20	0.8	0.18	0.76
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	20	0.8	0.44	0.7
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	20	0.79	0.05	0.78
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	20	0.79	0.12	0.82
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG11	20	0.79	0.02	0.79
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG13	20	0.79	0.02	0.79
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG12	20	0.79	0.02	0.79
(1,607)	1:36:A:THR:H	1:36:A:THR:HG22	20	0.79	0.17	0.79
(1,607)	1:36:A:THR:H	1:36:A:THR:HG23	20	0.79	0.17	0.79
(1,607)	1:36:A:THR:H	1:36:A:THR:HG21	20	0.79	0.17	0.79
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	20	0.78	0.04	0.79
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	20	0.78	0.19	0.76
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	20	0.78	0.27	0.82
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	20	0.78	0.13	0.76
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	20	0.78	0.07	0.79
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	20	0.78	0.05	0.78
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	20	0.77	0.28	0.82
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	20	0.77	0.01	0.77
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	20	0.77	0.17	0.73

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	20	0.77	0.13	0.77
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	20	0.77	0.25	0.88
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	20	0.76	0.25	0.76
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	20	0.76	0.09	0.76
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	20	0.76	0.43	0.63
(1,1402)	1:80:A:LEU:HD23	1:75:A:GLY:HA3	20	0.75	0.13	0.79
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	20	0.75	0.13	0.79
(1,1402)	1:80:A:LEU:HD22	1:75:A:GLY:HA3	20	0.75	0.13	0.79
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	20	0.75	0.44	0.51
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG22	20	0.75	0.3	0.64
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG23	20	0.75	0.3	0.64
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG21	20	0.75	0.3	0.64
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG11	20	0.74	0.16	0.74
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG13	20	0.74	0.16	0.74
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG12	20	0.74	0.16	0.74
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	20	0.74	0.19	0.78
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	20	0.74	0.45	0.6
(1,827)	1:51:A:LEU:HD13	1:51:A:LEU:H	20	0.74	0.16	0.72
(1,827)	1:51:A:LEU:HD11	1:51:A:LEU:H	20	0.74	0.16	0.72
(1,827)	1:51:A:LEU:HD12	1:51:A:LEU:H	20	0.74	0.16	0.72
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	20	0.73	0.16	0.79
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG22	20	0.72	0.36	0.69
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG23	20	0.72	0.36	0.69
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG21	20	0.72	0.36	0.69
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	20	0.72	0.03	0.72
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	20	0.71	0.02	0.72
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	20	0.71	0.07	0.72
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	20	0.71	0.27	0.66
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	20	0.71	0.08	0.7
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB2	20	0.7	0.1	0.7
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB3	20	0.7	0.1	0.7
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB1	20	0.7	0.1	0.7
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	20	0.7	0.12	0.68
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	20	0.7	0.13	0.66
(1,940)	1:59:A:VAL:HG12	1:66:A:LYS:HG2	20	0.7	0.33	0.64
(1,940)	1:59:A:VAL:HG11	1:66:A:LYS:HG2	20	0.7	0.33	0.64
(1,940)	1:59:A:VAL:HG13	1:66:A:LYS:HG2	20	0.7	0.33	0.64
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	20	0.7	0.26	0.86
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	20	0.7	0.08	0.7
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	20	0.69	0.07	0.69
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	20	0.69	0.24	0.66
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	20	0.69	0.02	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	20	0.68	0.16	0.68
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	20	0.68	0.19	0.76
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	20	0.68	0.34	0.6
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD11	20	0.68	0.34	0.6
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD12	20	0.68	0.34	0.6
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	20	0.67	0.01	0.68
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	20	0.66	0.02	0.66
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	20	0.66	0.13	0.68
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	20	0.66	0.15	0.61
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	20	0.65	0.14	0.66
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	20	0.65	0.23	0.58
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	20	0.65	0.03	0.64
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	20	0.64	0.37	0.57
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	20	0.64	0.04	0.64
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	20	0.64	0.18	0.59
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	20	0.64	0.04	0.62
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	20	0.64	0.15	0.64
(1,302)	1:18:A:THR:HG21	1:20:A:LYS:HD2	20	0.63	0.17	0.59
(1,302)	1:18:A:THR:HG22	1:20:A:LYS:HD2	20	0.63	0.17	0.59
(1,302)	1:18:A:THR:HG23	1:20:A:LYS:HD2	20	0.63	0.17	0.59
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	20	0.63	0.05	0.63
(1,828)	1:51:A:LEU:HD13	1:52:A:ASN:H	20	0.63	0.07	0.62
(1,828)	1:51:A:LEU:HD11	1:52:A:ASN:H	20	0.63	0.07	0.62
(1,828)	1:51:A:LEU:HD12	1:52:A:ASN:H	20	0.63	0.07	0.62
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	20	0.62	0.16	0.62
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	20	0.62	0.05	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	20	0.62	0.0	0.62
(1,310)	1:18:A:THR:H	1:18:A:THR:HG21	20	0.62	0.04	0.62
(1,310)	1:18:A:THR:H	1:18:A:THR:HG22	20	0.62	0.04	0.62
(1,310)	1:18:A:THR:H	1:18:A:THR:HG23	20	0.62	0.04	0.62
(1,1478)	1:18:A:THR:HG21	1:20:A:LYS:HB3	20	0.62	0.12	0.64
(1,1478)	1:18:A:THR:HG22	1:20:A:LYS:HB3	20	0.62	0.12	0.64
(1,1478)	1:18:A:THR:HG23	1:20:A:LYS:HB3	20	0.62	0.12	0.64
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	20	0.61	0.01	0.61
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	20	0.61	0.02	0.6
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	20	0.6	0.24	0.6
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	20	0.6	0.06	0.6
(1,822)	1:51:A:LEU:HD22	1:56:A:CYS:HB3	20	0.6	0.17	0.59
(1,822)	1:51:A:LEU:HD21	1:56:A:CYS:HB3	20	0.6	0.17	0.59
(1,822)	1:51:A:LEU:HD23	1:56:A:CYS:HB3	20	0.6	0.17	0.59
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	20	0.6	0.17	0.58
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	20	0.6	0.09	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	20	0.6	0.05	0.6
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	20	0.59	0.07	0.6
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	20	0.59	0.04	0.6
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	20	0.59	0.22	0.55
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	20	0.58	0.07	0.57
(1,695)	1:44:A:ALA:HB3	1:45:A:CYS:HB3	20	0.58	0.21	0.57
(1,695)	1:44:A:ALA:HB1	1:45:A:CYS:HB3	20	0.58	0.21	0.57
(1,695)	1:44:A:ALA:HB2	1:45:A:CYS:HB3	20	0.58	0.21	0.57
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	20	0.58	0.08	0.59
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	20	0.58	0.03	0.58
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	20	0.57	0.16	0.54
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	20	0.57	0.02	0.57
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	20	0.57	0.12	0.55
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	20	0.56	0.19	0.56
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	20	0.56	0.09	0.56
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	20	0.56	0.29	0.55
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	20	0.56	0.11	0.56
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	20	0.55	0.13	0.55
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	20	0.54	0.14	0.56
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	20	0.52	0.14	0.5
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	20	0.52	0.0	0.52
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	20	0.52	0.32	0.42
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	20	0.51	0.11	0.54
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	20	0.51	0.23	0.45
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	20	0.51	0.07	0.52
(1,872)	1:55:A:THR:HG21	1:67:A:CYS:HA	20	0.51	0.2	0.6
(1,872)	1:55:A:THR:HG23	1:67:A:CYS:HA	20	0.51	0.2	0.6
(1,872)	1:55:A:THR:HG22	1:67:A:CYS:HA	20	0.51	0.2	0.6
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	20	0.5	0.16	0.52
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	20	0.5	0.16	0.56
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG21	20	0.5	0.15	0.5
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG22	20	0.5	0.15	0.5
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG23	20	0.5	0.15	0.5
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD23	20	0.49	0.15	0.5
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	20	0.49	0.15	0.5
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD22	20	0.49	0.15	0.5
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	20	0.49	0.11	0.5
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	20	0.49	0.04	0.48
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	20	0.49	0.02	0.49
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	20	0.49	0.14	0.46
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	20	0.49	0.01	0.49
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	20	0.48	0.14	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	20	0.48	0.12	0.46
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	20	0.47	0.05	0.48
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	20	0.47	0.04	0.46
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	20	0.47	0.12	0.45
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	20	0.46	0.1	0.43
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	20	0.46	0.19	0.38
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	20	0.46	0.31	0.3
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	20	0.46	0.13	0.45
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	20	0.45	0.19	0.43
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	20	0.45	0.05	0.41
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	20	0.44	0.02	0.44
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	20	0.43	0.03	0.43
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	20	0.43	0.09	0.42
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	20	0.42	0.02	0.43
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	20	0.42	0.04	0.43
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	20	0.41	0.02	0.4
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	20	0.4	0.07	0.42
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	20	0.39	0.19	0.35
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	20	0.39	0.02	0.39
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	20	0.39	0.08	0.39
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	20	0.39	0.01	0.4
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	20	0.39	0.23	0.32
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	20	0.38	0.14	0.36
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	20	0.38	0.15	0.32
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	20	0.38	0.11	0.36
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	20	0.37	0.04	0.38
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	20	0.36	0.04	0.37
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	20	0.35	0.04	0.34
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	20	0.35	0.09	0.35
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	20	0.35	0.06	0.34
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	20	0.35	0.04	0.35
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	20	0.32	0.05	0.31
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	20	0.32	0.02	0.33
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	20	0.32	0.02	0.32
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	20	0.32	0.05	0.32
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	20	0.31	0.1	0.31
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	20	0.31	0.1	0.28
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	20	0.31	0.05	0.32
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	20	0.31	0.04	0.32
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	20	0.31	0.09	0.34
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	20	0.3	0.07	0.26
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	20	0.29	0.08	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	20	0.29	0.13	0.2
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	20	0.28	0.14	0.24
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG23	20	0.28	0.03	0.28
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG21	20	0.28	0.03	0.28
(1,938)	1:59:A:VAL:HG11	1:59:A:VAL:HG21	20	0.28	0.03	0.28
(1,938)	1:59:A:VAL:HG11	1:59:A:VAL:HG22	20	0.28	0.03	0.28
(1,938)	1:59:A:VAL:HG13	1:59:A:VAL:HG21	20	0.28	0.03	0.28
(1,938)	1:59:A:VAL:HG11	1:59:A:VAL:HG23	20	0.28	0.03	0.28
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG22	20	0.28	0.03	0.28
(1,938)	1:59:A:VAL:HG13	1:59:A:VAL:HG23	20	0.28	0.03	0.28
(1,938)	1:59:A:VAL:HG13	1:59:A:VAL:HG22	20	0.28	0.03	0.28
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	20	0.28	0.04	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	20	0.28	0.0	0.28
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	20	0.27	0.04	0.26
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	20	0.26	0.03	0.25
(1,1317)	1:80:A:LEU:HD22	1:80:A:LEU:HD13	20	0.26	0.01	0.26
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD11	20	0.26	0.01	0.26
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD12	20	0.26	0.01	0.26
(1,1317)	1:80:A:LEU:HD21	1:80:A:LEU:HD13	20	0.26	0.01	0.26
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD13	20	0.26	0.01	0.26
(1,1317)	1:80:A:LEU:HD21	1:80:A:LEU:HD11	20	0.26	0.01	0.26
(1,1317)	1:80:A:LEU:HD22	1:80:A:LEU:HD11	20	0.26	0.01	0.26
(1,1317)	1:80:A:LEU:HD22	1:80:A:LEU:HD12	20	0.26	0.01	0.26
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	20	0.25	0.03	0.26
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	20	0.25	0.06	0.27
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	20	0.25	0.05	0.26
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	20	0.24	0.04	0.22
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	20	0.24	0.01	0.24
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	20	0.23	0.05	0.22
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	20	0.22	0.04	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	20	0.22	0.01	0.22
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	20	0.22	0.04	0.22
(1,826)	1:51:A:LEU:HD11	1:51:A:LEU:HD23	20	0.22	0.01	0.22
(1,826)	1:51:A:LEU:HD11	1:51:A:LEU:HD21	20	0.22	0.01	0.22
(1,826)	1:51:A:LEU:HD11	1:51:A:LEU:HD22	20	0.22	0.01	0.22
(1,826)	1:51:A:LEU:HD12	1:51:A:LEU:HD23	20	0.22	0.01	0.22
(1,826)	1:51:A:LEU:HD13	1:51:A:LEU:HD21	20	0.22	0.01	0.22
(1,826)	1:51:A:LEU:HD13	1:51:A:LEU:HD22	20	0.22	0.01	0.22
(1,826)	1:51:A:LEU:HD12	1:51:A:LEU:HD21	20	0.22	0.01	0.22
(1,826)	1:51:A:LEU:HD13	1:51:A:LEU:HD23	20	0.22	0.01	0.22
(1,826)	1:51:A:LEU:HD12	1:51:A:LEU:HD22	20	0.22	0.01	0.22
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	20	0.22	0.04	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1863)	1:68:A:SER:HB3	1:67:A:CYS:HB3	20	0.21	0.06	0.22
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	20	0.17	0.06	0.15
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	20	0.13	0.0	0.13
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG21	19	2.32	1.48	1.51
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG22	19	2.32	1.48	1.51
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG23	19	2.32	1.48	1.51
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	19	2.12	1.04	2.27
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	19	1.88	0.29	1.82
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	19	1.74	0.53	2.05
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	19	1.73	0.7	1.62
(1,697)	1:44:A:ALA:HB3	1:34:A:GLY:HA2	19	1.41	0.62	1.5
(1,697)	1:44:A:ALA:HB2	1:34:A:GLY:HA2	19	1.41	0.62	1.5
(1,697)	1:44:A:ALA:HB1	1:34:A:GLY:HA2	19	1.41	0.62	1.5
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	19	1.24	0.67	1.13
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	19	1.13	0.53	1.18
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG23	19	1.12	0.35	1.11
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG21	19	1.12	0.35	1.11
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG22	19	1.12	0.35	1.11
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	19	1.11	0.37	1.09
(1,599)	1:36:A:THR:HG23	1:64:A:TYR:HB3	19	1.09	0.49	1.08
(1,599)	1:36:A:THR:HG22	1:64:A:TYR:HB3	19	1.09	0.49	1.08
(1,599)	1:36:A:THR:HG21	1:64:A:TYR:HB3	19	1.09	0.49	1.08
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	19	1.02	0.03	1.03
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	19	1.01	0.5	1.0
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	19	1.0	0.44	0.94
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	19	0.99	0.19	1.0
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	19	0.98	0.13	0.93
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG13	19	0.97	0.45	0.91
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG12	19	0.97	0.45	0.91
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG11	19	0.97	0.45	0.91
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	19	0.9	0.35	0.96
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	19	0.86	0.19	0.86
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	19	0.85	0.15	0.85
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	19	0.8	0.29	0.87
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	19	0.78	0.01	0.77
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	19	0.75	0.42	0.77
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	19	0.73	0.16	0.77
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	19	0.68	0.23	0.79
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	19	0.66	0.38	0.92
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	19	0.66	0.3	0.64
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	19	0.61	0.28	0.63
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	19	0.61	0.15	0.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	19	0.6	0.25	0.6
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	19	0.58	0.16	0.63
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	19	0.57	0.03	0.57
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	19	0.57	0.4	0.44
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	19	0.56	0.02	0.56
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	19	0.55	0.21	0.58
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	19	0.52	0.02	0.52
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	19	0.46	0.16	0.42
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	19	0.45	0.11	0.43
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	19	0.43	0.34	0.25
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	19	0.42	0.08	0.4
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	19	0.42	0.01	0.42
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	19	0.41	0.01	0.42
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	19	0.41	0.27	0.29
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	19	0.41	0.0	0.41
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	19	0.41	0.11	0.41
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	19	0.4	0.1	0.45
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	19	0.4	0.18	0.4
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	19	0.36	0.13	0.36
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	19	0.35	0.32	0.29
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	19	0.35	0.04	0.36
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	19	0.33	0.05	0.33
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	19	0.32	0.01	0.32
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	19	0.31	0.09	0.29
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	19	0.3	0.04	0.3
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	19	0.25	0.05	0.26
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	19	0.21	0.03	0.22
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	19	0.16	0.01	0.17
(1,7)	1:28:A:LYS:HA	1:27:A:TYR:HA	19	0.13	0.02	0.13
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	19	0.13	0.02	0.13
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD21	18	1.18	0.3	1.19
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD22	18	1.18	0.3	1.19
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD23	18	1.18	0.3	1.19
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	18	1.08	0.88	0.87
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	18	1.0	0.64	0.92
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	18	0.93	0.31	0.92
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	18	0.84	0.33	0.76
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD11	18	0.82	0.3	0.75
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD12	18	0.82	0.3	0.75
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD13	18	0.82	0.3	0.75
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	18	0.75	0.14	0.78
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	18	0.71	0.31	0.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG23	18	0.71	0.15	0.66
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG21	18	0.71	0.15	0.66
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG22	18	0.71	0.15	0.66
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	18	0.68	0.3	0.64
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	18	0.66	0.28	0.66
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	18	0.61	0.32	0.58
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	18	0.6	0.02	0.6
(1,1500)	1:51:A:LEU:HD21	1:50:A:CYS:H	18	0.59	0.27	0.6
(1,1500)	1:51:A:LEU:HD22	1:50:A:CYS:H	18	0.59	0.27	0.6
(1,1500)	1:51:A:LEU:HD23	1:50:A:CYS:H	18	0.59	0.27	0.6
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	18	0.58	0.15	0.57
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	18	0.55	0.18	0.54
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	18	0.53	0.19	0.58
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	18	0.51	0.34	0.46
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	18	0.51	0.17	0.48
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG13	18	0.49	0.19	0.49
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG12	18	0.49	0.19	0.49
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG11	18	0.49	0.19	0.49
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	18	0.49	0.26	0.68
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	18	0.48	0.18	0.42
(1,824)	1:51:A:LEU:HD21	1:51:A:LEU:H	18	0.46	0.17	0.44
(1,824)	1:51:A:LEU:HD22	1:51:A:LEU:H	18	0.46	0.17	0.44
(1,824)	1:51:A:LEU:HD23	1:51:A:LEU:H	18	0.46	0.17	0.44
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	18	0.46	0.09	0.47
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	18	0.45	0.28	0.31
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	18	0.44	0.19	0.36
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	18	0.42	0.3	0.32
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	18	0.42	0.41	0.26
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	18	0.42	0.21	0.36
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	18	0.41	0.11	0.38
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	18	0.38	0.15	0.38
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	18	0.37	0.16	0.4
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	18	0.35	0.13	0.34
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	18	0.34	0.16	0.3
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	18	0.32	0.21	0.22
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	18	0.28	0.12	0.24
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	18	0.25	0.04	0.25
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	18	0.19	0.05	0.2
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	18	0.19	0.05	0.16
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	18	0.15	0.02	0.16
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	17	2.39	0.76	2.44
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	17	0.97	0.33	1.01

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	17	0.96	0.69	0.66
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	17	0.9	0.6	0.71
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	17	0.84	0.17	0.85
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	17	0.77	0.08	0.77
(1,698)	1:44:A:ALA:HB2	1:65:A:TYR:HB2	17	0.75	0.13	0.73
(1,698)	1:44:A:ALA:HB3	1:65:A:TYR:HB2	17	0.75	0.13	0.73
(1,698)	1:44:A:ALA:HB1	1:65:A:TYR:HB2	17	0.75	0.13	0.73
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	17	0.7	0.39	0.73
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	17	0.7	0.04	0.7
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	17	0.65	0.19	0.62
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	17	0.59	0.04	0.58
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	17	0.55	0.42	0.41
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	17	0.52	0.05	0.52
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	17	0.46	0.2	0.49
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD12	17	0.46	0.2	0.38
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD13	17	0.46	0.2	0.38
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD11	17	0.46	0.2	0.38
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	17	0.42	0.19	0.39
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	17	0.42	0.35	0.24
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	17	0.36	0.19	0.33
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	17	0.34	0.12	0.37
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	17	0.32	0.14	0.31
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	17	0.3	0.32	0.2
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	17	0.29	0.0	0.29
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	17	0.29	0.04	0.29
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	17	0.23	0.03	0.24
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	17	0.22	0.04	0.24
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	17	0.21	0.1	0.18
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	17	0.2	0.08	0.18
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	17	0.12	0.01	0.12
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	16	1.32	1.1	0.81
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	16	1.25	0.08	1.24
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HD2	16	1.25	0.08	1.24
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE2	16	0.91	0.49	0.9
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE3	16	0.91	0.49	0.9
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	16	0.74	0.33	0.7
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	16	0.73	0.16	0.73
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	16	0.72	0.41	0.76
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	16	0.69	0.13	0.68
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	16	0.68	0.19	0.76
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	16	0.53	0.26	0.54
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	16	0.48	0.25	0.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	16	0.48	0.29	0.38
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	16	0.47	0.26	0.44
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	16	0.33	0.17	0.24
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	16	0.29	0.11	0.3
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	16	0.27	0.14	0.22
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	16	0.24	0.05	0.23
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	16	0.23	0.21	0.13
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	16	0.22	0.08	0.22
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	16	0.2	0.06	0.19
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	16	0.11	0.0	0.11
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	15	1.51	0.52	1.65
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	15	1.12	0.22	1.12
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	15	0.92	0.72	0.66
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	15	0.85	0.35	0.84
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	15	0.81	0.75	0.43
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD22	15	0.72	0.58	0.45
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD11	15	0.72	0.58	0.45
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD23	15	0.72	0.58	0.45
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD13	15	0.72	0.58	0.45
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD21	15	0.72	0.58	0.45
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD12	15	0.72	0.58	0.45
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	15	0.69	0.59	0.47
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	15	0.63	0.4	0.57
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	15	0.58	0.33	0.6
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	15	0.54	0.31	0.47
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	15	0.51	0.27	0.48
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	15	0.5	0.0	0.5
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	15	0.49	0.0	0.49
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	15	0.48	0.35	0.38
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	15	0.47	0.54	0.33
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	15	0.46	0.24	0.43
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	15	0.44	0.26	0.39
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	15	0.44	0.2	0.4
(1,1036)	1:59:A:VAL:HG11	1:65:A:TYR:HA	15	0.37	0.16	0.34
(1,1036)	1:59:A:VAL:HG13	1:65:A:TYR:HA	15	0.37	0.16	0.34
(1,1036)	1:59:A:VAL:HG12	1:65:A:TYR:HA	15	0.37	0.16	0.34
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	15	0.37	0.12	0.39
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	15	0.32	0.27	0.17
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	15	0.29	0.16	0.23
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	15	0.23	0.12	0.17
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	15	0.21	0.09	0.19
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	15	0.19	0.03	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	14	1.17	0.3	1.14
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	14	1.1	0.57	1.0
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	14	1.01	1.1	0.8
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	14	0.75	0.29	0.69
(1,15)	1:40:A:CYS:HB2	1:32:A:ARG:HB3	14	0.75	0.29	0.69
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	14	0.66	0.3	0.56
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	14	0.64	0.26	0.67
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	14	0.59	0.24	0.5
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG13	14	0.54	0.25	0.53
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG12	14	0.54	0.25	0.53
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG11	14	0.54	0.25	0.53
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	14	0.53	0.14	0.54
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	14	0.53	0.18	0.57
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	14	0.45	0.28	0.39
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	14	0.4	0.28	0.4
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	14	0.38	0.36	0.22
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	14	0.33	0.15	0.35
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	14	0.32	0.16	0.28
(1,705)	1:44:A:ALA:HB3	1:65:A:TYR:HA	14	0.29	0.16	0.27
(1,705)	1:44:A:ALA:HB2	1:65:A:TYR:HA	14	0.29	0.16	0.27
(1,705)	1:44:A:ALA:HB1	1:65:A:TYR:HA	14	0.29	0.16	0.27
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	14	0.28	0.3	0.16
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	14	0.27	0.13	0.23
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	14	0.25	0.11	0.23
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	14	0.21	0.06	0.2
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	14	0.2	0.03	0.2
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	14	0.19	0.05	0.18
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	14	0.17	0.16	0.13
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	14	0.17	0.04	0.16
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	14	0.14	0.03	0.14
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	13	1.51	0.6	1.24
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	13	1.22	0.44	1.37
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	13	1.21	0.51	1.11
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	13	0.87	0.58	0.75
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	13	0.86	0.2	0.9
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	13	0.85	0.29	0.84
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	13	0.78	0.35	0.95
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	13	0.64	0.03	0.65
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	13	0.62	0.39	0.57
(1,1436)	1:44:A:ALA:HB3	1:58:A:TYR:HE1	13	0.6	0.29	0.43
(1,1436)	1:44:A:ALA:HB2	1:58:A:TYR:HE1	13	0.6	0.29	0.43
(1,1436)	1:44:A:ALA:HB1	1:58:A:TYR:HE1	13	0.6	0.29	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG12	13	0.58	0.01	0.58
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG13	13	0.58	0.01	0.58
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG11	13	0.58	0.01	0.58
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	13	0.55	0.39	0.37
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	13	0.53	0.05	0.54
(1,960)	1:59:A:VAL:HG22	1:60:A:TYR:HB2	13	0.49	0.47	0.21
(1,960)	1:59:A:VAL:HG21	1:60:A:TYR:HB2	13	0.49	0.47	0.21
(1,960)	1:59:A:VAL:HG23	1:60:A:TYR:HB2	13	0.49	0.47	0.21
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	13	0.49	0.22	0.47
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	13	0.45	0.03	0.47
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	13	0.44	0.22	0.42
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	13	0.37	0.12	0.38
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	13	0.33	0.0	0.33
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	13	0.3	0.14	0.31
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	13	0.28	0.08	0.25
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	13	0.26	0.13	0.22
(1,1477)	1:18:A:THR:HG21	1:19:A:CYS:HB3	13	0.23	0.09	0.22
(1,1477)	1:18:A:THR:HG22	1:19:A:CYS:HB3	13	0.23	0.09	0.22
(1,1477)	1:18:A:THR:HG23	1:19:A:CYS:HB3	13	0.23	0.09	0.22
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	13	0.21	0.18	0.17
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	13	0.2	0.0	0.2
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	13	0.19	0.01	0.19
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	13	0.15	0.01	0.15
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	13	0.14	0.02	0.14
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	12	0.96	0.75	0.72
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	12	0.9	0.32	1.1
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	12	0.73	0.07	0.74
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	12	0.69	0.42	0.59
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	12	0.68	0.33	0.82
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	12	0.64	0.29	0.82
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	12	0.53	0.22	0.55
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	12	0.49	0.23	0.44
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	12	0.46	0.15	0.44
(1,707)	1:44:A:ALA:HB3	1:58:A:TYR:HD1	12	0.38	0.19	0.38
(1,707)	1:44:A:ALA:HB2	1:58:A:TYR:HD1	12	0.38	0.19	0.38
(1,707)	1:44:A:ALA:HB1	1:58:A:TYR:HD1	12	0.38	0.19	0.38
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	12	0.34	0.09	0.35
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	12	0.3	0.32	0.12
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	12	0.3	0.13	0.32
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	12	0.24	0.16	0.19
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	12	0.22	0.07	0.21
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	12	0.19	0.14	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	12	0.18	0.05	0.18
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	12	0.15	0.03	0.15
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	11	1.42	0.22	1.42
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG12	11	1.22	0.9	1.65
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG11	11	1.22	0.9	1.65
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG13	11	1.22	0.9	1.65
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	11	1.09	0.37	0.86
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	11	0.78	0.38	0.71
(1,12)	1:34:A:GLY:HA3	1:58:A:TYR:HB3	11	0.7	0.44	0.59
(1,12)	1:34:A:GLY:HA3	1:33:A:LYS:HE2	11	0.7	0.44	0.59
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	11	0.6	0.32	0.62
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	11	0.58	0.27	0.72
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	11	0.48	0.31	0.34
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG12	11	0.46	0.3	0.32
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG13	11	0.46	0.3	0.32
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG11	11	0.46	0.3	0.32
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	11	0.43	0.0	0.43
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	11	0.38	0.28	0.25
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	11	0.37	0.13	0.43
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	11	0.34	0.16	0.29
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	11	0.32	0.13	0.3
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	11	0.26	0.1	0.3
(1,597)	1:36:A:THR:HG21	1:42:A:TYR:HB3	11	0.25	0.14	0.25
(1,597)	1:36:A:THR:HG22	1:42:A:TYR:HB3	11	0.25	0.14	0.25
(1,597)	1:36:A:THR:HG23	1:42:A:TYR:HB3	11	0.25	0.14	0.25
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	11	0.21	0.08	0.2
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG13	11	0.21	0.06	0.2
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG12	11	0.21	0.06	0.2
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG11	11	0.21	0.06	0.2
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	11	0.18	0.07	0.18
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	11	0.18	0.07	0.17
(1,43)	1:2:A:VAL:HG23	1:4:A:TYR:HD1	10	1.71	0.91	2.22
(1,43)	1:2:A:VAL:HG22	1:4:A:TYR:HD1	10	1.71	0.91	2.22
(1,43)	1:2:A:VAL:HG21	1:4:A:TYR:HD1	10	1.71	0.91	2.22
(1,1185)	1:72:A:GLY:HA3	1:71:A:TYR:HD1	10	1.29	0.35	1.29
(1,1166)	1:71:A:TYR:HA	1:71:A:TYR:HD1	10	0.79	0.15	0.77
(1,1182)	1:72:A:GLY:HA2	1:71:A:TYR:HD1	10	0.74	0.33	0.83
(1,61)	1:71:A:TYR:HE1	1:71:A:TYR:HA	10	0.59	0.14	0.58
(1,1337)	1:81:A:LYS:HB2	1:83:A:TYR:HE1	10	0.52	0.44	0.34
(1,175)	1:8:A:CYS:H	1:7:A:PRO:HD2	10	0.44	0.21	0.48
(1,60)	1:71:A:TYR:HD1	1:71:A:TYR:HB3	10	0.42	0.01	0.42
(1,212)	1:10:A:PRO:HA	1:9:A:SER:H	10	0.36	0.14	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1603)	1:29:A:CYS:H	1:28:A:LYS:HE3	10	0.34	0.16	0.3
(1,1740)	1:57:A:GLY:H	1:66:A:LYS:HB2	10	0.33	0.16	0.3
(1,588)	1:58:A:TYR:HB2	1:59:A:VAL:H	10	0.32	0.12	0.34
(1,1776)	1:65:A:TYR:H	1:59:A:VAL:HB	10	0.28	0.16	0.25
(1,1703)	1:45:A:CYS:H	1:58:A:TYR:HD1	10	0.24	0.12	0.21
(1,849)	1:54:A:GLY:HA2	1:70:A:PRO:HD2	10	0.23	0.09	0.22
(1,59)	1:71:A:TYR:HD1	1:71:A:TYR:HB2	10	0.23	0.03	0.24
(1,1696)	1:44:A:ALA:H	1:43:A:ASN:HB2	10	0.22	0.04	0.22
(1,1133)	1:71:A:TYR:H	1:70:A:PRO:HB2	10	0.19	0.07	0.18
(1,1683)	1:42:A:TYR:H	1:42:A:TYR:HB3	10	0.17	0.03	0.17
(1,1426)	1:53:A:GLY:HA2	1:52:A:ASN:H	10	0.16	0.06	0.15
(1,1400)	1:76:A:LYS:HD2	1:76:A:LYS:HE2	10	0.15	0.0	0.15
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG21	9	1.44	0.91	1.8
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG22	9	1.44	0.91	1.8
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG23	9	1.44	0.91	1.8
(1,1071)	1:67:A:CYS:HA	1:50:A:CYS:HB3	9	1.41	0.67	1.75
(1,183)	1:7:A:PRO:HG3	1:21:A:LYS:HG3	9	0.95	0.63	0.88
(1,483)	1:28:A:LYS:HB3	1:28:A:LYS:HE2	9	0.8	0.21	0.81
(1,617)	1:38:A:LYS:HA	1:38:A:LYS:HE3	9	0.68	0.43	0.61
(1,365)	1:21:A:LYS:HE2	1:21:A:LYS:HD3	9	0.6	0.01	0.6
(1,641)	1:39:A:ASN:HA	1:29:A:CYS:HB3	9	0.6	0.46	0.49
(1,38)	1:82:A:LYS:H	1:74:A:TYR:HE1	9	0.45	0.27	0.41
(1,636)	1:38:A:LYS:HG3	1:38:A:LYS:HA	9	0.39	0.05	0.42
(1,1671)	1:41:A:GLN:H	1:39:A:ASN:HB3	9	0.39	0.22	0.36
(1,1191)	1:73:A:TYR:HB3	1:70:A:PRO:HD3	9	0.34	0.17	0.33
(1,1131)	1:70:A:PRO:HB3	1:73:A:TYR:HD1	9	0.28	0.18	0.23
(1,1886)	1:22:A:ARG:H	1:27:A:TYR:HD1	9	0.27	0.12	0.23
(1,1676)	1:79:A:GLN:H	1:75:A:GLY:HA2	9	0.27	0.09	0.24
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG11	9	0.26	0.13	0.21
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG12	9	0.26	0.13	0.21
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG13	9	0.26	0.13	0.21
(1,1572)	1:23:A:GLY:H	1:22:A:ARG:HB2	9	0.26	0.06	0.27
(1,85)	1:3:A:TYR:HA	1:2:A:VAL:HG21	8	1.97	0.64	2.2
(1,85)	1:3:A:TYR:HA	1:2:A:VAL:HG23	8	1.97	0.64	2.2
(1,85)	1:3:A:TYR:HA	1:2:A:VAL:HG22	8	1.97	0.64	2.2
(1,1228)	1:75:A:GLY:HA3	1:76:A:LYS:HG3	8	0.88	0.7	0.86
(1,1379)	1:82:A:LYS:HE2	1:74:A:TYR:HE1	8	0.84	0.53	0.94
(1,1602)	1:29:A:CYS:H	1:28:A:LYS:HD2	8	0.81	0.67	0.37
(1,256)	1:14:A:ARG:HD2	1:14:A:ARG:H	8	0.75	0.26	0.84
(1,787)	1:49:A:PRO:HD3	1:48:A:ASN:HB3	8	0.73	0.11	0.76
(1,488)	1:28:A:LYS:HE2	1:28:A:LYS:HA	8	0.72	0.61	0.58
(1,84)	1:3:A:TYR:H	1:2:A:VAL:HG21	8	0.69	0.09	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,84)	1:3:A:TYR:H	1:2:A:VAL:HG23	8	0.69	0.09	0.68
(1,84)	1:3:A:TYR:H	1:2:A:VAL:HG22	8	0.69	0.09	0.68
(1,83)	1:2:A:VAL:HG22	1:4:A:TYR:HE1	8	0.65	0.29	0.64
(1,83)	1:2:A:VAL:HG21	1:4:A:TYR:HE1	8	0.65	0.29	0.64
(1,83)	1:2:A:VAL:HG23	1:4:A:TYR:HE1	8	0.65	0.29	0.64
(1,307)	1:18:A:THR:HG22	1:30:A:TYR:HE1	8	0.63	0.35	0.56
(1,307)	1:18:A:THR:HG21	1:30:A:TYR:HE1	8	0.63	0.35	0.56
(1,307)	1:18:A:THR:HG23	1:30:A:TYR:HE1	8	0.63	0.35	0.56
(1,1698)	1:44:A:ALA:H	1:58:A:TYR:HE1	8	0.56	0.26	0.54
(1,600)	1:36:A:THR:HG21	1:64:A:TYR:HB2	8	0.5	0.29	0.41
(1,600)	1:36:A:THR:HG22	1:64:A:TYR:HB2	8	0.5	0.29	0.41
(1,600)	1:36:A:THR:HG23	1:64:A:TYR:HB2	8	0.5	0.29	0.41
(1,1539)	1:17:A:GLY:H	1:32:A:ARG:HG2	8	0.46	0.52	0.21
(1,1620)	1:31:A:CYS:H	1:18:A:THR:HB	8	0.44	0.11	0.43
(1,623)	1:38:A:LYS:HB3	1:38:A:LYS:HE2	8	0.42	0.2	0.46
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD21	8	0.4	0.21	0.38
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD13	8	0.4	0.21	0.38
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD12	8	0.4	0.21	0.38
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD11	8	0.4	0.21	0.38
(1,1347)	1:82:A:LYS:HA	1:82:A:LYS:HG2	8	0.39	0.37	0.28
(1,699)	1:44:A:ALA:HB3	1:64:A:TYR:HB3	8	0.3	0.2	0.24
(1,699)	1:44:A:ALA:HB1	1:64:A:TYR:HB3	8	0.3	0.2	0.24
(1,699)	1:44:A:ALA:HB2	1:64:A:TYR:HB3	8	0.3	0.2	0.24
(1,304)	1:18:A:THR:HG22	1:30:A:TYR:HB2	8	0.29	0.14	0.26
(1,304)	1:18:A:THR:HG21	1:30:A:TYR:HB2	8	0.29	0.14	0.26
(1,96)	1:3:A:TYR:HB2	1:3:A:TYR:H	8	0.28	0.22	0.19
(1,664)	1:40:A:CYS:HB2	1:31:A:CYS:HA	8	0.26	0.13	0.24
(1,1417)	1:63:A:PRO:HB2	1:64:A:TYR:HD1	8	0.24	0.1	0.22
(1,1709)	1:46:A:PHE:H	1:46:A:PHE:HD1	8	0.23	0.11	0.2
(1,1357)	1:82:A:LYS:HB2	1:82:A:LYS:HG2	8	0.22	0.01	0.22
(1,1635)	1:34:A:GLY:H	1:33:A:LYS:HB3	8	0.17	0.05	0.16
(1,683)	1:43:A:ASN:HA	1:44:A:ALA:HA	8	0.14	0.02	0.13
(1,1755)	1:59:A:VAL:H	1:60:A:TYR:H	8	0.14	0.02	0.13
(1,1874)	1:34:A:GLY:H	1:33:A:LYS:HB2	8	0.12	0.01	0.12
(1,771)	1:49:A:PRO:HA	1:49:A:PRO:HG3	8	0.11	0.01	0.12
(1,1506)	1:4:A:TYR:H	1:2:A:VAL:HG23	7	2.25	0.21	2.26
(1,1506)	1:4:A:TYR:H	1:2:A:VAL:HG22	7	2.25	0.21	2.26
(1,1506)	1:4:A:TYR:H	1:2:A:VAL:HG21	7	2.25	0.21	2.26
(1,497)	1:67:A:CYS:HB2	1:50:A:CYS:HB3	7	1.24	0.14	1.23
(1,23)	1:78:A:CYS:HB2	1:70:A:PRO:HD3	7	1.09	0.39	1.06
(1,564)	1:34:A:GLY:HA3	1:58:A:TYR:HE1	7	0.98	0.53	0.74
(1,1882)	1:2:A:VAL:H	1:2:A:VAL:HG11	7	0.89	0.06	0.87

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1882)	1:2:A:VAL:H	1:2:A:VAL:HG13	7	0.89	0.06	0.87
(1,9)	1:31:A:CYS:HB2	1:32:A:ARG:HG2	7	0.82	0.22	0.86
(1,9)	1:31:A:CYS:HB2	1:32:A:ARG:HB3	7	0.82	0.22	0.86
(1,216)	1:10:A:PRO:HB2	1:10:A:PRO:HD2	7	0.78	0.01	0.78
(1,752)	1:47:A:PRO:HD2	1:47:A:PRO:HB2	7	0.7	0.01	0.71
(1,1459)	1:14:A:ARG:HG2	1:14:A:ARG:HD2	7	0.63	0.0	0.63
(1,736)	1:47:A:PRO:HA	1:47:A:PRO:HG3	7	0.5	0.04	0.5
(1,297)	1:18:A:THR:HB	1:30:A:TYR:HE1	7	0.44	0.27	0.3
(1,592)	1:36:A:THR:HB	1:44:A:ALA:HB2	7	0.41	0.31	0.27
(1,592)	1:36:A:THR:HB	1:44:A:ALA:HB3	7	0.41	0.31	0.27
(1,592)	1:36:A:THR:HB	1:44:A:ALA:HB1	7	0.41	0.31	0.27
(1,455)	1:27:A:TYR:HA	1:21:A:LYS:HB2	7	0.38	0.41	0.18
(1,6)	1:7:A:PRO:HD2	1:21:A:LYS:HE3	7	0.38	0.21	0.32
(1,6)	1:7:A:PRO:HD2	1:27:A:TYR:HB2	7	0.38	0.21	0.32
(1,802)	1:50:A:CYS:H	1:50:A:CYS:HB2	7	0.35	0.02	0.35
(1,117)	1:5:A:PRO:HB2	1:5:A:PRO:HD2	7	0.35	0.05	0.35
(1,688)	1:44:A:ALA:HA	1:36:A:THR:HG23	7	0.31	0.16	0.29
(1,688)	1:44:A:ALA:HA	1:36:A:THR:HG21	7	0.31	0.16	0.29
(1,688)	1:44:A:ALA:HA	1:36:A:THR:HG22	7	0.31	0.16	0.29
(1,1486)	1:7:A:PRO:HD3	1:6:A:ASN:HB3	7	0.3	0.13	0.36
(1,1510)	1:6:A:ASN:H	1:5:A:PRO:HB2	7	0.3	0.11	0.32
(1,1658)	1:39:A:ASN:H	1:41:A:GLN:H	7	0.27	0.09	0.21
(1,751)	1:47:A:PRO:HD3	1:47:A:PRO:HG2	7	0.26	0.01	0.26
(1,549)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	7	0.26	0.08	0.2
(1,1619)	1:31:A:CYS:H	1:30:A:TYR:HB2	7	0.24	0.05	0.26
(1,1159)	1:70:A:PRO:HG3	1:55:A:THR:H	7	0.2	0.13	0.13
(1,958)	1:66:A:LYS:H	1:59:A:VAL:HG11	7	0.2	0.07	0.21
(1,958)	1:66:A:LYS:H	1:59:A:VAL:HG12	7	0.2	0.07	0.21
(1,958)	1:66:A:LYS:H	1:59:A:VAL:HG13	7	0.2	0.07	0.21
(1,1754)	1:59:A:VAL:H	1:58:A:TYR:HD1	7	0.2	0.09	0.17
(1,1810)	1:73:A:TYR:H	1:81:A:LYS:HA	7	0.19	0.11	0.14
(1,1512)	1:6:A:ASN:H	1:6:A:ASN:HB3	7	0.18	0.05	0.17
(1,1809)	1:73:A:TYR:H	1:72:A:GLY:HA3	7	0.15	0.03	0.14
(1,1419)	1:60:A:TYR:HA	1:59:A:VAL:HG22	7	0.14	0.05	0.11
(1,1419)	1:60:A:TYR:HA	1:59:A:VAL:HG23	7	0.14	0.05	0.11
(1,1419)	1:60:A:TYR:HA	1:59:A:VAL:HG21	7	0.14	0.05	0.11
(1,1777)	1:65:A:TYR:H	1:65:A:TYR:HB2	7	0.12	0.01	0.12
(1,614)	1:38:A:LYS:HA	1:38:A:LYS:HG2	6	0.54	0.45	0.46
(1,1319)	1:79:A:GLN:HG3	1:80:A:LEU:HD23	6	0.53	0.39	0.36
(1,1319)	1:79:A:GLN:HG3	1:80:A:LEU:HD21	6	0.53	0.39	0.36
(1,1398)	1:78:A:CYS:HA	1:69:A:CYS:HB3	6	0.44	0.25	0.3
(1,478)	1:66:A:LYS:HB2	1:66:A:LYS:HE2	6	0.4	0.2	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,181)	1:7:A:PRO:HG2	1:27:A:TYR:HA	6	0.33	0.22	0.26
(1,393)	1:22:A:ARG:HG3	1:28:A:LYS:H	6	0.31	0.25	0.24
(1,1666)	1:79:A:GLN:H	1:80:A:LEU:HD11	6	0.29	0.11	0.26
(1,1666)	1:79:A:GLN:H	1:80:A:LEU:HD12	6	0.29	0.11	0.26
(1,704)	1:44:A:ALA:HB3	1:35:A:TYR:HA	6	0.25	0.16	0.22
(1,704)	1:44:A:ALA:HB1	1:35:A:TYR:HA	6	0.25	0.16	0.22
(1,704)	1:44:A:ALA:HB2	1:35:A:TYR:HA	6	0.25	0.16	0.22
(1,603)	1:36:A:THR:HG22	1:42:A:TYR:HA	6	0.25	0.12	0.26
(1,603)	1:36:A:THR:HG23	1:42:A:TYR:HA	6	0.25	0.12	0.26
(1,603)	1:36:A:THR:HG21	1:42:A:TYR:HA	6	0.25	0.12	0.26
(1,804)	1:51:A:LEU:H	1:50:A:CYS:HB3	6	0.25	0.06	0.24
(1,1636)	1:34:A:GLY:H	1:35:A:TYR:HD1	6	0.23	0.1	0.19
(1,230)	1:10:A:PRO:HG3	1:11:A:TYR:H	6	0.21	0.06	0.2
(1,219)	1:11:A:TYR:H	1:10:A:PRO:HB2	6	0.21	0.04	0.21
(1,489)	1:29:A:CYS:HA	1:18:A:THR:HG21	6	0.18	0.07	0.16
(1,489)	1:29:A:CYS:HA	1:18:A:THR:HG22	6	0.18	0.07	0.16
(1,489)	1:29:A:CYS:HA	1:18:A:THR:HG23	6	0.18	0.07	0.16
(1,199)	1:9:A:SER:H	1:9:A:SER:HB3	6	0.18	0.03	0.18
(1,392)	1:22:A:ARG:HG3	1:22:A:ARG:H	6	0.17	0.04	0.17
(1,1571)	1:82:A:LYS:H	1:74:A:TYR:HD1	6	0.16	0.04	0.16
(1,1579)	1:24:A:LEU:H	1:25:A:TYR:HA	6	0.16	0.04	0.16
(2,12)	1:55:A:THR:N	1:68:A:SER:O	6	0.11	0.01	0.11
(1,166)	1:7:A:PRO:HD3	1:21:A:LYS:HG3	5	1.22	0.24	1.33
(1,1645)	1:35:A:TYR:H	1:33:A:LYS:HG2	5	0.95	0.4	1.13
(1,1064)	1:66:A:LYS:HG3	1:59:A:VAL:HG23	5	0.86	0.63	0.79
(1,1064)	1:66:A:LYS:HG3	1:59:A:VAL:HG21	5	0.86	0.63	0.79
(1,1857)	1:83:A:TYR:H	1:82:A:LYS:HG2	5	0.8	0.44	0.6
(1,24)	1:78:A:CYS:HB3	1:70:A:PRO:HD3	5	0.68	0.22	0.7
(1,401)	1:23:A:GLY:HA3	1:24:A:LEU:HD22	5	0.67	0.33	0.7
(1,401)	1:23:A:GLY:HA3	1:24:A:LEU:HD23	5	0.67	0.33	0.7
(1,401)	1:23:A:GLY:HA3	1:24:A:LEU:HD21	5	0.67	0.33	0.7
(1,412)	1:24:A:LEU:H	1:24:A:LEU:HD22	5	0.66	0.12	0.65
(1,412)	1:24:A:LEU:H	1:24:A:LEU:HD23	5	0.66	0.12	0.65
(1,412)	1:24:A:LEU:H	1:24:A:LEU:HD21	5	0.66	0.12	0.65
(1,1050)	1:65:A:TYR:HB3	1:58:A:TYR:HA	5	0.66	0.31	0.74
(1,633)	1:66:A:LYS:HE2	1:66:A:LYS:HG3	5	0.63	0.44	0.78
(1,635)	1:38:A:LYS:HG3	1:38:A:LYS:HE2	5	0.62	0.2	0.52
(1,988)	1:62:A:TYR:HA	1:62:A:TYR:HD1	5	0.53	0.36	0.36
(1,551)	1:33:A:LYS:HB3	1:33:A:LYS:HE2	5	0.44	0.15	0.53
(1,891)	1:57:A:GLY:HA2	1:66:A:LYS:HB2	5	0.36	0.16	0.39
(1,573)	1:73:A:TYR:HA	1:81:A:LYS:HG2	5	0.33	0.14	0.29
(1,666)	1:40:A:CYS:HB2	1:39:A:ASN:HA	5	0.33	0.05	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,286)	1:18:A:THR:HA	1:30:A:TYR:HD1	5	0.33	0.18	0.3
(1,550)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	5	0.31	0.04	0.28
(1,1047)	1:58:A:TYR:H	1:65:A:TYR:HA	5	0.3	0.11	0.37
(1,480)	1:28:A:LYS:HB2	1:22:A:ARG:H	5	0.28	0.09	0.32
(1,150)	1:6:A:ASN:HA	1:21:A:LYS:HG3	5	0.26	0.05	0.27
(1,1281)	1:79:A:GLN:HG2	1:80:A:LEU:HB2	5	0.26	0.13	0.19
(1,565)	1:34:A:GLY:HA3	1:35:A:TYR:HD1	5	0.25	0.13	0.22
(1,10)	1:31:A:CYS:HB2	1:32:A:ARG:HA	5	0.23	0.09	0.18
(1,875)	1:68:A:SER:H	1:55:A:THR:HG22	5	0.19	0.05	0.22
(1,875)	1:68:A:SER:H	1:55:A:THR:HG21	5	0.19	0.05	0.22
(1,875)	1:68:A:SER:H	1:55:A:THR:HG23	5	0.19	0.05	0.22
(1,62)	1:73:A:TYR:HD1	1:73:A:TYR:HA	5	0.15	0.03	0.16
(1,1843)	1:78:A:CYS:H	1:77:A:GLN:HB2	5	0.13	0.02	0.14
(1,330)	1:20:A:LYS:HB2	1:20:A:LYS:HD3	5	0.12	0.01	0.11
(1,127)	1:5:A:PRO:HD2	1:5:A:PRO:HA	5	0.11	0.01	0.11
(1,387)	1:22:A:ARG:HA	1:22:A:ARG:HD2	4	1.66	0.76	2.09
(1,560)	1:34:A:GLY:HA2	1:33:A:LYS:HG2	4	1.12	0.44	1.06
(1,559)	1:33:A:LYS:HG2	1:34:A:GLY:HA3	4	1.04	0.51	0.85
(1,1207)	1:75:A:GLY:HA2	1:76:A:LYS:HG3	4	0.86	0.05	0.84
(1,235)	1:11:A:TYR:HA	1:11:A:TYR:HD1	4	0.85	0.13	0.9
(1,249)	1:13:A:CYS:HB2	1:11:A:TYR:HD1	4	0.82	0.46	0.72
(1,1634)	1:34:A:GLY:H	1:33:A:LYS:HG2	4	0.82	0.22	0.77
(1,1467)	1:22:A:ARG:HD2	1:22:A:ARG:H	4	0.81	0.13	0.79
(1,1373)	1:72:A:GLY:HA2	1:82:A:LYS:HD2	4	0.64	0.35	0.73
(1,176)	1:7:A:PRO:HG2	1:21:A:LYS:HG3	4	0.62	0.41	0.55
(1,1745)	1:57:A:GLY:H	1:65:A:TYR:HD1	4	0.6	0.41	0.52
(1,1860)	1:83:A:TYR:H	1:74:A:TYR:HD1	4	0.58	0.3	0.62
(1,1103)	1:69:A:CYS:HB2	1:78:A:CYS:HA	4	0.55	0.31	0.54
(1,1046)	1:59:A:VAL:H	1:65:A:TYR:HA	4	0.5	0.34	0.48
(1,762)	1:48:A:ASN:HA	1:49:A:PRO:HB3	4	0.44	0.2	0.52
(1,1829)	1:76:A:LYS:H	1:76:A:LYS:HG3	4	0.42	0.04	0.42
(1,532)	1:32:A:ARG:HD2	1:32:A:ARG:H	4	0.35	0.2	0.27
(1,510)	1:31:A:CYS:HB2	1:40:A:CYS:HB2	4	0.34	0.3	0.19
(1,1800)	1:72:A:GLY:H	1:82:A:LYS:HB3	4	0.28	0.25	0.14
(1,490)	1:29:A:CYS:HA	1:20:A:LYS:HG2	4	0.26	0.17	0.2
(1,1869)	1:53:A:GLY:H	1:51:A:LEU:HD22	4	0.26	0.08	0.24
(1,1869)	1:53:A:GLY:H	1:51:A:LEU:HD23	4	0.26	0.08	0.24
(1,1869)	1:53:A:GLY:H	1:51:A:LEU:HD21	4	0.26	0.08	0.24
(1,516)	1:32:A:ARG:HA	1:35:A:TYR:HD1	4	0.24	0.1	0.23
(1,391)	1:22:A:ARG:HG3	1:27:A:TYR:HA	4	0.21	0.08	0.19
(1,237)	1:11:A:TYR:HB3	1:11:A:TYR:H	4	0.2	0.05	0.22
(1,816)	1:51:A:LEU:HB3	1:52:A:ASN:HA	4	0.18	0.05	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1226)	1:76:A:LYS:HA	1:75:A:GLY:H	4	0.18	0.03	0.18
(1,1844)	1:78:A:CYS:H	1:74:A:TYR:HA	4	0.18	0.03	0.18
(1,396)	1:22:A:ARG:HG2	1:22:A:ARG:HA	4	0.15	0.02	0.16
(1,1122)	1:70:A:PRO:HB2	1:70:A:PRO:HD3	4	0.14	0.02	0.14
(1,1826)	1:75:A:GLY:H	1:77:A:GLN:H	4	0.13	0.01	0.13
(1,404)	1:23:A:GLY:HA3	1:22:A:ARG:HA	4	0.11	0.01	0.11
(1,115)	1:6:A:ASN:H	1:5:A:PRO:HA	3	1.09	0.02	1.08
(1,239)	1:13:A:CYS:HA	1:14:A:ARG:HG2	3	1.05	0.75	1.01
(1,647)	1:39:A:ASN:HB2	1:41:A:GLN:HB3	3	0.93	0.33	1.07
(1,1789)	1:67:A:CYS:H	1:65:A:TYR:HD1	3	0.9	0.11	0.92
(1,453)	1:22:A:ARG:HG2	1:27:A:TYR:HA	3	0.86	0.21	0.77
(1,1300)	1:79:A:GLN:HG3	1:80:A:LEU:HB2	3	0.81	0.35	1.04
(1,978)	1:60:A:TYR:H	1:60:A:TYR:HB2	3	0.73	0.04	0.7
(1,103)	1:4:A:TYR:HB2	1:4:A:TYR:HD1	3	0.72	0.05	0.73
(1,344)	1:18:A:THR:HG22	1:20:A:LYS:HE2	3	0.63	0.32	0.41
(1,344)	1:18:A:THR:HG23	1:20:A:LYS:HE2	3	0.63	0.32	0.41
(1,347)	1:20:A:LYS:HG2	1:20:A:LYS:HE2	3	0.63	0.0	0.63
(1,527)	1:32:A:ARG:HD2	1:32:A:ARG:HG2	3	0.62	0.0	0.62
(1,976)	1:60:A:TYR:HB2	1:60:A:TYR:HD1	3	0.62	0.04	0.61
(1,116)	1:63:A:PRO:HB2	1:63:A:PRO:HD2	3	0.56	0.0	0.56
(1,122)	1:5:A:PRO:HB3	1:3:A:TYR:HE1	3	0.56	0.22	0.67
(1,1454)	1:33:A:LYS:HG2	1:33:A:LYS:HE3	3	0.56	0.05	0.58
(1,838)	1:53:A:GLY:HA2	1:70:A:PRO:HG3	3	0.53	0.39	0.42
(1,262)	1:15:A:ASN:HB3	1:35:A:TYR:HD1	3	0.53	0.27	0.54
(1,555)	1:33:A:LYS:HE2	1:33:A:LYS:HG2	3	0.51	0.01	0.52
(1,1469)	1:22:A:ARG:HB3	1:22:A:ARG:HD2	3	0.5	0.08	0.45
(1,798)	1:50:A:CYS:HA	1:77:A:GLN:HA	3	0.45	0.09	0.47
(1,648)	1:39:A:ASN:HB2	1:41:A:GLN:HB2	3	0.44	0.19	0.34
(1,1540)	1:17:A:GLY:H	1:13:A:CYS:HB2	3	0.41	0.16	0.35
(1,1056)	1:66:A:LYS:H	1:65:A:TYR:HB2	3	0.38	0.02	0.37
(1,477)	1:28:A:LYS:HB2	1:28:A:LYS:HE3	3	0.34	0.09	0.39
(1,1015)	1:64:A:TYR:H	1:63:A:PRO:HG3	3	0.32	0.02	0.33
(1,1821)	1:74:A:TYR:H	1:74:A:TYR:HE1	3	0.32	0.3	0.11
(1,569)	1:34:A:GLY:HA2	1:58:A:TYR:HD1	3	0.32	0.09	0.31
(1,380)	1:22:A:ARG:HB2	1:22:A:ARG:HG2	3	0.31	0.0	0.31
(1,1527)	1:14:A:ARG:H	1:39:A:ASN:HA	3	0.27	0.07	0.24
(1,1762)	1:61:A:GLY:H	1:60:A:TYR:HB2	3	0.26	0.07	0.24
(1,605)	1:37:A:GLY:H	1:36:A:THR:HG23	3	0.26	0.05	0.27
(1,605)	1:37:A:GLY:H	1:36:A:THR:HG22	3	0.26	0.05	0.27
(1,48)	1:24:A:LEU:HB3	1:25:A:TYR:HE1	3	0.24	0.03	0.24
(1,493)	1:29:A:CYS:HA	1:30:A:TYR:HD1	3	0.21	0.05	0.23
(1,994)	1:63:A:PRO:HA	1:63:A:PRO:HG3	3	0.21	0.02	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,717)	1:45:A:CYS:HA	1:58:A:TYR:HE1	3	0.21	0.07	0.2
(1,1030)	1:64:A:TYR:HB3	1:65:A:TYR:HB3	3	0.16	0.04	0.16
(1,1713)	1:48:A:ASN:H	1:49:A:PRO:HD2	3	0.15	0.03	0.16
(1,1220)	1:76:A:LYS:HA	1:76:A:LYS:HG2	3	0.15	0.02	0.14
(1,252)	1:16:A:GLY:H	1:14:A:ARG:HA	3	0.14	0.04	0.12
(1,265)	1:15:A:ASN:HB2	1:35:A:TYR:HD1	3	0.13	0.01	0.14
(1,485)	1:66:A:LYS:HB3	1:65:A:TYR:HA	3	0.12	0.01	0.13
(1,385)	1:22:A:ARG:HB3	1:22:A:ARG:H	3	0.11	0.01	0.11
(1,509)	1:31:A:CYS:H	1:31:A:CYS:HB3	3	0.11	0.01	0.1
(1,961)	1:59:A:VAL:HA	1:59:A:VAL:HG23	3	0.1	0.0	0.1
(1,961)	1:59:A:VAL:HA	1:59:A:VAL:HG22	3	0.1	0.0	0.1
(1,939)	1:59:A:VAL:HG12	1:66:A:LYS:HG3	2	1.08	0.6	1.08
(1,939)	1:59:A:VAL:HG13	1:66:A:LYS:HG3	2	1.08	0.6	1.08
(1,1508)	1:4:A:TYR:H	1:4:A:TYR:HD1	2	0.84	0.3	0.84
(1,123)	1:5:A:PRO:HB3	1:3:A:TYR:HD1	2	0.82	0.65	0.82
(1,1418)	1:62:A:TYR:HB3	1:62:A:TYR:HD1	2	0.79	0.02	0.79
(1,437)	1:25:A:TYR:HB2	1:26:A:SER:HB2	2	0.78	0.09	0.78
(1,568)	1:34:A:GLY:HA2	1:58:A:TYR:HE1	2	0.74	0.58	0.74
(1,1523)	1:14:A:ARG:H	1:14:A:ARG:HG2	2	0.72	0.44	0.72
(1,1292)	1:80:A:LEU:HA	1:79:A:GLN:HG3	2	0.66	0.23	0.66
(1,1437)	1:44:A:ALA:HB2	1:36:A:THR:HG22	2	0.66	0.27	0.66
(1,1437)	1:44:A:ALA:HB2	1:36:A:THR:HG23	2	0.66	0.27	0.66
(1,794)	1:50:A:CYS:HA	1:77:A:GLN:HG2	2	0.62	0.17	0.62
(1,841)	1:53:A:GLY:HA3	1:70:A:PRO:HG2	2	0.58	0.11	0.58
(1,1110)	1:69:A:CYS:HB2	1:75:A:GLY:H	2	0.57	0.01	0.57
(1,1493)	1:2:A:VAL:HG12	1:4:A:TYR:HD1	2	0.57	0.46	0.57
(1,1493)	1:2:A:VAL:HG11	1:4:A:TYR:HD1	2	0.57	0.46	0.57
(1,1246)	1:77:A:GLN:HA	1:77:A:GLN:HG2	2	0.54	0.0	0.54
(1,1410)	1:70:A:PRO:HG2	1:54:A:GLY:H	2	0.51	0.21	0.51
(1,660)	1:40:A:CYS:HB3	1:35:A:TYR:HB3	2	0.49	0.0	0.49
(1,314)	1:19:A:CYS:HB3	1:11:A:TYR:HE1	2	0.48	0.28	0.48
(1,1804)	1:72:A:GLY:H	1:71:A:TYR:HD1	2	0.46	0.0	0.46
(1,1756)	1:59:A:VAL:H	1:66:A:LYS:H	2	0.46	0.08	0.46
(1,645)	1:39:A:ASN:HB3	1:41:A:GLN:HB3	2	0.44	0.06	0.44
(1,1054)	1:65:A:TYR:HB2	1:58:A:TYR:HD1	2	0.42	0.26	0.42
(1,955)	1:61:A:GLY:H	1:59:A:VAL:HG13	2	0.4	0.05	0.4
(1,308)	1:18:A:THR:HG21	1:30:A:TYR:HD1	2	0.38	0.16	0.38
(1,308)	1:18:A:THR:HG22	1:30:A:TYR:HD1	2	0.38	0.16	0.38
(1,1684)	1:42:A:TYR:H	1:39:A:ASN:HB2	2	0.38	0.03	0.38
(1,206)	1:9:A:SER:H	1:9:A:SER:HB2	2	0.34	0.01	0.34
(1,983)	1:62:A:TYR:HA	1:59:A:VAL:HG13	2	0.32	0.06	0.32
(1,606)	1:44:A:ALA:H	1:36:A:THR:HG22	2	0.32	0.22	0.32

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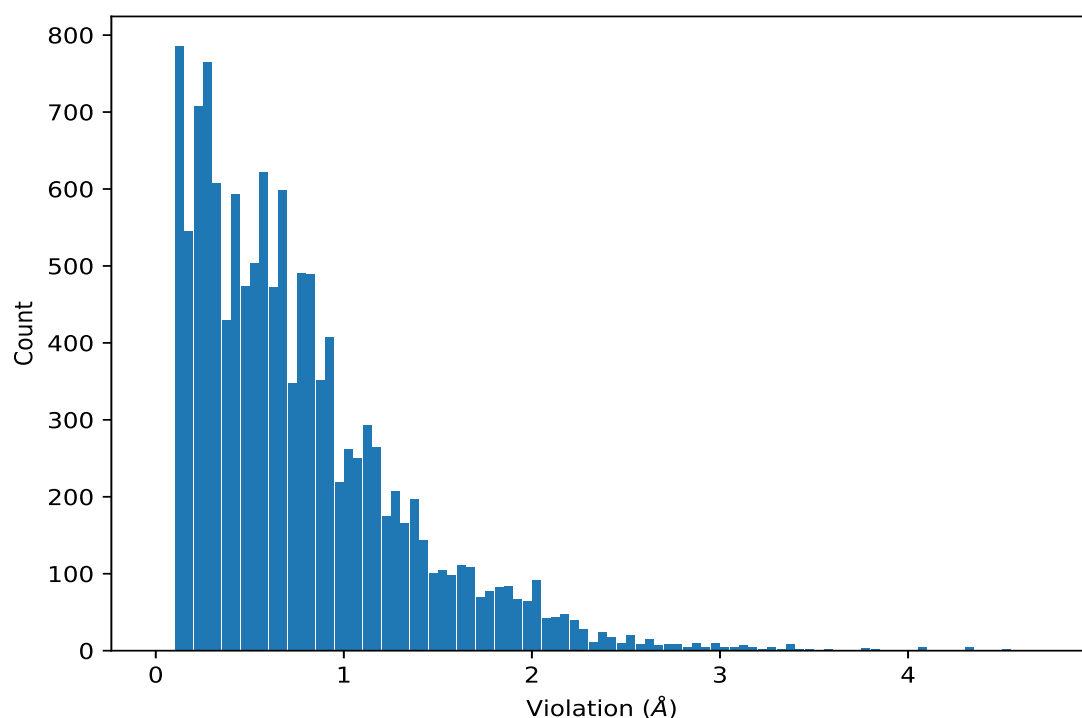
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,606)	1:44:A:ALA:H	1:36:A:THR:HG23	2	0.32	0.22	0.32
(1,906)	1:58:A:TYR:HA	1:65:A:TYR:HB2	2	0.32	0.18	0.32
(1,1413)	1:28:A:LYS:HA	1:28:A:LYS:HB2	2	0.32	0.19	0.32
(1,1381)	1:82:A:LYS:HG2	1:74:A:TYR:HE1	2	0.32	0.16	0.32
(1,792)	1:50:A:CYS:HA	1:77:A:GLN:HG3	2	0.31	0.14	0.31
(1,134)	1:4:A:TYR:H	1:5:A:PRO:HD3	2	0.3	0.15	0.3
(1,1580)	1:24:A:LEU:H	1:25:A:TYR:HD1	2	0.26	0.13	0.26
(1,434)	1:26:A:SER:H	1:25:A:TYR:HB3	2	0.25	0.07	0.25
(1,946)	1:59:A:VAL:HG13	1:61:A:GLY:HA3	2	0.24	0.12	0.24
(1,1353)	1:82:A:LYS:HA	1:74:A:TYR:HD1	2	0.22	0.12	0.22
(1,1514)	1:6:A:ASN:H	1:7:A:PRO:HD2	2	0.22	0.07	0.22
(1,194)	1:8:A:CYS:HB2	1:7:A:PRO:HA	2	0.19	0.06	0.19
(1,1146)	1:70:A:PRO:HD2	1:73:A:TYR:HA	2	0.18	0.04	0.18
(1,35)	1:80:A:LEU:H	1:79:A:GLN:HB2	2	0.18	0.08	0.18
(1,1714)	1:50:A:CYS:H	1:49:A:PRO:HG2	2	0.18	0.04	0.18
(1,700)	1:44:A:ALA:HB1	1:64:A:TYR:HB2	2	0.16	0.01	0.16
(1,1640)	1:35:A:TYR:H	1:36:A:THR:HA	2	0.16	0.04	0.16
(1,1751)	1:59:A:VAL:H	1:66:A:LYS:HB2	2	0.16	0.01	0.16
(1,182)	1:7:A:PRO:HG2	1:27:A:TYR:HD1	2	0.15	0.02	0.15
(1,818)	1:51:A:LEU:H	1:51:A:LEU:HB3	2	0.15	0.0	0.15
(1,46)	1:11:A:TYR:HE1	1:11:A:TYR:HB3	2	0.14	0.04	0.14
(1,1513)	1:6:A:ASN:H	1:7:A:PRO:HD3	2	0.14	0.0	0.14
(1,245)	1:13:A:CYS:HA	1:39:A:ASN:HA	2	0.13	0.0	0.13
(1,315)	1:19:A:CYS:HB3	1:11:A:TYR:HD1	2	0.13	0.01	0.13
(1,1752)	1:59:A:VAL:H	1:64:A:TYR:HB3	2	0.13	0.03	0.13
(1,768)	1:48:A:ASN:HA	1:50:A:CYS:H	2	0.12	0.01	0.12
(1,1009)	1:63:A:PRO:HD2	1:63:A:PRO:HA	2	0.12	0.0	0.12
(1,1656)	1:39:A:ASN:H	1:37:A:GLY:HA2	2	0.12	0.0	0.12
(1,1716)	1:50:A:CYS:H	1:49:A:PRO:HD3	2	0.12	0.0	0.12
(1,57)	1:64:A:TYR:HE1	1:63:A:PRO:HA	2	0.11	0.01	0.11
(1,850)	1:54:A:GLY:HA2	1:69:A:CYS:HA	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	5	4.75
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	12	4.54
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG21	10	4.5
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG21	2	4.36
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	3	4.35
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG21	1	4.33
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG21	19	4.31
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	10	4.3
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	6	4.1
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG23	4	4.1
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	9	4.08
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG22	11	4.08
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG23	8	4.05
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG21	4	3.94
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG21	11	3.86
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG22	8	3.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG23	10	3.82
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	5	3.8
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	6	3.77
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	8	3.77
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	19	3.7
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG22	19	3.6
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	11	3.59
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	13	3.59
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	5	3.48
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG22	1	3.48
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	19	3.44
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	12	3.42
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	8	3.4
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG21	12	3.4
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	16	3.38
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	3	3.38
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG22	2	3.38
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	5	3.37
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	17	3.37
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	2	3.37
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	20	3.35
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	7	3.34
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	2	3.34
(1,1028)	1:59:A:VAL:HG11	1:64:A:TYR:HB3	14	3.29
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	18	3.28
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	9	3.27
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	19	3.27
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	9	3.25
(1,1027)	1:59:A:VAL:HG11	1:64:A:TYR:HB2	14	3.24
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	20	3.22
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	19	3.18
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	12	3.17
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	6	3.16
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	16	3.16
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	18	3.16
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	8	3.15
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	16	3.14
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	11	3.14
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	5	3.14
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	5	3.11
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	16	3.11
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	4	3.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	4	3.09
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	13	3.08
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	17	3.08
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	19	3.08
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	13	3.07
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	18	3.05
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	17	3.04
(1,694)	1:44:A:ALA:HB3	1:59:A:VAL:HG11	14	3.01
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	3	3.01
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	5	2.99
(1,1028)	1:59:A:VAL:HG11	1:64:A:TYR:HB3	11	2.98
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	15	2.98
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	10	2.98
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	4	2.97
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	20	2.97
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	7	2.97
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	7	2.97
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	2	2.96
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	16	2.96
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	19	2.94
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	14	2.92
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	16	2.92
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	7	2.91
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	13	2.91
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	19	2.89
(1,1027)	1:59:A:VAL:HG11	1:64:A:TYR:HB2	11	2.89
(1,1005)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	14	2.89
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	9	2.89
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	17	2.88
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	10	2.87
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	1	2.86
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	1	2.86
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	8	2.85
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	16	2.85
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	13	2.84
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	17	2.81
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	1	2.81
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	6	2.81
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	12	2.8
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	17	2.8
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	11	2.79
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	7	2.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG13	14	2.78
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	18	2.78
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	5	2.77
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	14	2.76
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	20	2.76
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	4	2.74
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	8	2.73
(1,948)	1:59:A:VAL:HG13	1:64:A:TYR:HA	14	2.73
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG12	17	2.73
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	14	2.73
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	1	2.73
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	13	2.71
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	3	2.71
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	12	2.67
(1,694)	1:44:A:ALA:HB1	1:59:A:VAL:HG13	13	2.67
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	15	2.67
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	7	2.67
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	19	2.67
(1,1028)	1:59:A:VAL:HG13	1:64:A:TYR:HB3	13	2.66
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	6	2.66
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	13	2.65
(1,1028)	1:59:A:VAL:HG13	1:64:A:TYR:HB3	8	2.65
(1,1028)	1:59:A:VAL:HG11	1:64:A:TYR:HB3	16	2.65
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG11	11	2.65
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG11	14	2.65
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	13	2.64
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	9	2.64
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	12	2.64
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	9	2.63
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	12	2.63
(1,1028)	1:59:A:VAL:HG12	1:64:A:TYR:HB3	5	2.63
(1,1005)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	11	2.63
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	12	2.63
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	17	2.63
(1,694)	1:44:A:ALA:HB1	1:59:A:VAL:HG11	11	2.62
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	2	2.59
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	10	2.59
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	19	2.57
(1,1028)	1:59:A:VAL:HG12	1:64:A:TYR:HB3	17	2.57
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	3	2.57
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG12	5	2.57
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	4	2.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1027)	1:59:A:VAL:HG13	1:64:A:TYR:HB2	13	2.56
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	13	2.56
(1,504)	1:30:A:TYR:HB3	1:18:A:THR:HA	12	2.55
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	6	2.55
(1,43)	1:2:A:VAL:HG22	1:4:A:TYR:HD1	11	2.55
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	6	2.54
(1,1506)	1:4:A:TYR:H	1:2:A:VAL:HG22	8	2.53
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	4	2.53
(1,694)	1:44:A:ALA:HB1	1:59:A:VAL:HG13	19	2.53
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG23	12	2.53
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	14	2.53
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG13	8	2.52
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	9	2.51
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	18	2.51
(1,1027)	1:59:A:VAL:HG11	1:64:A:TYR:HB2	16	2.51
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG13	11	2.51
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	8	2.51
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG13	13	2.51
(1,694)	1:44:A:ALA:HB3	1:59:A:VAL:HG12	17	2.51
(1,382)	1:22:A:ARG:HB3	1:26:A:SER:HB2	15	2.51
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	3	2.5
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	20	2.5
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	12	2.49
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	13	2.49
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	10	2.48
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG22	11	2.48
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	20	2.48
(1,948)	1:59:A:VAL:HG11	1:64:A:TYR:HA	11	2.47
(1,43)	1:2:A:VAL:HG23	1:4:A:TYR:HD1	10	2.47
(1,694)	1:44:A:ALA:HB3	1:59:A:VAL:HG13	7	2.46
(1,1027)	1:59:A:VAL:HG12	1:64:A:TYR:HB2	5	2.45
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG11	16	2.45
(1,1506)	1:4:A:TYR:H	1:2:A:VAL:HG23	4	2.44
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	11	2.44
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	20	2.44
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	3	2.44
(1,962)	1:59:A:VAL:HG21	1:65:A:TYR:H	14	2.44
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	20	2.44
(1,1506)	1:4:A:TYR:H	1:2:A:VAL:HG21	10	2.43
(1,1028)	1:59:A:VAL:HG13	1:64:A:TYR:HB3	15	2.43
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG13	15	2.43
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	20	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	9	2.43
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	15	2.42
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	20	2.42
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	17	2.42
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	7	2.41
(1,1028)	1:59:A:VAL:HG13	1:64:A:TYR:HB3	7	2.41
(1,694)	1:44:A:ALA:HB2	1:59:A:VAL:HG13	8	2.41
(1,43)	1:2:A:VAL:HG23	1:4:A:TYR:HD1	8	2.41
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	2	2.4
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG11	3	2.4
(1,1027)	1:59:A:VAL:HG13	1:64:A:TYR:HB2	8	2.4
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG23	17	2.4
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	5	2.4
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	18	2.39
(1,1027)	1:59:A:VAL:HG12	1:64:A:TYR:HB2	17	2.39
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG23	18	2.38
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	14	2.38
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	2	2.38
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	9	2.38
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	8	2.37
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	4	2.37
(1,18)	1:59:A:VAL:HG13	1:60:A:TYR:HB2	16	2.37
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	15	2.36
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	12	2.36
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG11	2	2.36
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	12	2.36
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	20	2.36
(1,26)	1:79:A:GLN:HB2	1:49:A:PRO:HA	3	2.36
(1,962)	1:59:A:VAL:HG22	1:65:A:TYR:H	11	2.35
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	4	2.35
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	20	2.35
(1,43)	1:2:A:VAL:HG21	1:4:A:TYR:HD1	4	2.35
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	14	2.34
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	7	2.34
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	10	2.34
(1,694)	1:44:A:ALA:HB3	1:59:A:VAL:HG12	5	2.34
(1,43)	1:2:A:VAL:HG22	1:4:A:TYR:HD1	19	2.34
(1,1027)	1:59:A:VAL:HG13	1:64:A:TYR:HB2	7	2.33
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	4	2.33
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	9	2.33
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	17	2.31
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	14	2.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	17	2.31
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG13	3	2.3
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	9	2.29
(1,697)	1:44:A:ALA:HB3	1:34:A:GLY:HA2	20	2.29
(1,694)	1:44:A:ALA:HB3	1:59:A:VAL:HG11	16	2.29
(1,694)	1:44:A:ALA:HB2	1:59:A:VAL:HG12	18	2.29
(1,694)	1:44:A:ALA:HB3	1:59:A:VAL:HG11	20	2.29
(1,183)	1:7:A:PRO:HG3	1:21:A:LYS:HG3	16	2.29
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	7	2.28
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG11	8	2.28
(1,694)	1:44:A:ALA:HB1	1:59:A:VAL:HG13	15	2.28
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	16	2.28
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	1	2.27
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	5	2.27
(1,85)	1:3:A:TYR:HA	1:2:A:VAL:HG21	1	2.27
(1,85)	1:3:A:TYR:HA	1:2:A:VAL:HG22	10	2.27
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	6	2.27
(1,1506)	1:4:A:TYR:H	1:2:A:VAL:HG23	1	2.26
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	11	2.26
(1,1027)	1:59:A:VAL:HG13	1:64:A:TYR:HB2	15	2.26
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	6	2.26
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	8	2.26
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	8	2.25
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	10	2.25
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	2	2.25
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	13	2.25
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	2	2.25
(1,488)	1:28:A:LYS:HE2	1:28:A:LYS:HA	2	2.25
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	13	2.25
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	9	2.24
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	19	2.24
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	10	2.24
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	11	2.24
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG13	7	2.24
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG21	3	2.24
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	17	2.23
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	15	2.23
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	3	2.23
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	17	2.23
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	6	2.23
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	15	2.23
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	17	2.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	13	2.23
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	2	2.23
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	7	2.22
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	12	2.22
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	2	2.22
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	4	2.22
(1,1028)	1:59:A:VAL:HG12	1:64:A:TYR:HB3	18	2.22
(1,694)	1:44:A:ALA:HB2	1:59:A:VAL:HG13	3	2.22
(1,694)	1:44:A:ALA:HB2	1:59:A:VAL:HG12	10	2.22
(1,18)	1:59:A:VAL:HG13	1:60:A:TYR:HB2	14	2.22
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	17	2.21
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	19	2.21
(1,1028)	1:59:A:VAL:HG12	1:64:A:TYR:HB3	10	2.21
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	10	2.21
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	7	2.21
(1,85)	1:3:A:TYR:HA	1:2:A:VAL:HG21	2	2.21
(1,85)	1:3:A:TYR:HA	1:2:A:VAL:HG21	19	2.21
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	7	2.21
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	14	2.2
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG23	2	2.2
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD22	11	2.2
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	12	2.2
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	19	2.2
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG12	18	2.2
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	15	2.2
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	18	2.2
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	19	2.2
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	8	2.19
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	2	2.19
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG21	20	2.19
(1,948)	1:59:A:VAL:HG12	1:64:A:TYR:HA	5	2.19
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	8	2.18
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	15	2.18
(1,1028)	1:59:A:VAL:HG13	1:64:A:TYR:HB3	20	2.18
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG23	5	2.18
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	3	2.18
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	9	2.18
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	13	2.18
(1,85)	1:3:A:TYR:HA	1:2:A:VAL:HG23	4	2.18
(1,85)	1:3:A:TYR:HA	1:2:A:VAL:HG22	8	2.18
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	13	2.18
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG22	9	2.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,962)	1:59:A:VAL:HG23	1:65:A:TYR:H	15	2.17
(1,867)	1:55:A:THR:HG23	1:54:A:GLY:HA2	7	2.17
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	1	2.17
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	6	2.17
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	8	2.17
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	12	2.17
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	14	2.17
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	6	2.16
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	8	2.16
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	14	2.16
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	12	2.16
(1,1028)	1:59:A:VAL:HG11	1:64:A:TYR:HB3	2	2.16
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	4	2.16
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	13	2.16
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	16	2.16
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	19	2.16
(1,85)	1:3:A:TYR:HA	1:2:A:VAL:HG21	11	2.16
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	16	2.15
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	19	2.15
(1,1506)	1:4:A:TYR:H	1:2:A:VAL:HG21	11	2.15
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG22	4	2.15
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	3	2.15
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	16	2.15
(1,1027)	1:59:A:VAL:HG12	1:64:A:TYR:HB2	18	2.15
(1,962)	1:59:A:VAL:HG22	1:65:A:TYR:H	16	2.15
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG12	10	2.15
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG13	12	2.15
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG23	20	2.15
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	2	2.15
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	7	2.15
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	11	2.15
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	20	2.15
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	20	2.14
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD23	13	2.14
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	20	2.14
(1,948)	1:59:A:VAL:HG11	1:64:A:TYR:HA	16	2.14
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	1	2.14
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	14	2.14
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	10	2.14
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	9	2.14
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	12	2.14
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE3	5	2.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	4	2.13
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD23	13	2.13
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD23	18	2.13
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG13	14	2.13
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	5	2.13
(1,731)	1:46:A:PHE:HB3	1:47:A:PRO:HA	19	2.13
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	7	2.13
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	10	2.13
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	11	2.13
(1,387)	1:22:A:ARG:HA	1:22:A:ARG:HD2	6	2.13
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	19	2.13
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	18	2.12
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	9	2.12
(1,965)	1:59:A:VAL:HG21	1:64:A:TYR:H	14	2.12
(1,948)	1:59:A:VAL:HG12	1:64:A:TYR:HA	13	2.12
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	20	2.12
(1,697)	1:44:A:ALA:HB2	1:34:A:GLY:HA2	13	2.12
(1,599)	1:36:A:THR:HG22	1:64:A:TYR:HB3	3	2.12
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	9	2.12
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	18	2.11
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	17	2.11
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD22	5	2.11
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	12	2.11
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	7	2.11
(1,948)	1:59:A:VAL:HG13	1:64:A:TYR:HA	8	2.11
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	17	2.11
(1,43)	1:2:A:VAL:HG23	1:4:A:TYR:HD1	1	2.11
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	15	2.11
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	11	2.11
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	14	2.1
(1,697)	1:44:A:ALA:HB3	1:34:A:GLY:HA2	14	2.1
(1,694)	1:44:A:ALA:HB1	1:59:A:VAL:HG13	4	2.1
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	10	2.1
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	18	2.1
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	8	2.09
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	4	2.09
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	5	2.09
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG12	15	2.09
(1,952)	1:59:A:VAL:HG11	1:58:A:TYR:HD1	14	2.09
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG11	1	2.09
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	3	2.09
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	1	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:22:A:ARG:HA	1:22:A:ARG:HD2	3	2.09
(1,387)	1:22:A:ARG:HA	1:22:A:ARG:HD2	5	2.09
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	20	2.09
(1,18)	1:59:A:VAL:HG12	1:60:A:TYR:HB2	13	2.09
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	9	2.08
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	6	2.08
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	17	2.08
(1,1028)	1:59:A:VAL:HG13	1:64:A:TYR:HB3	12	2.08
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG22	11	2.08
(1,952)	1:59:A:VAL:HG11	1:58:A:TYR:HD1	11	2.08
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG13	4	2.08
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG11	20	2.08
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	15	2.08
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	5	2.08
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	8	2.08
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	16	2.08
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD23	17	2.07
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	5	2.07
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	11	2.07
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG12	8	2.07
(1,962)	1:59:A:VAL:HG23	1:65:A:TYR:H	3	2.07
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG13	19	2.07
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG22	10	2.07
(1,867)	1:55:A:THR:HG22	1:54:A:GLY:HA2	11	2.07
(1,564)	1:34:A:GLY:HA3	1:58:A:TYR:HE1	14	2.07
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	17	2.07
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	4	2.07
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	11	2.07
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	1	2.06
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	11	2.06
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD22	19	2.06
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG21	12	2.06
(1,867)	1:55:A:THR:HG22	1:54:A:GLY:HA2	5	2.06
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	1	2.06
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	12	2.05
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD22	11	2.05
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	1	2.05
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	6	2.05
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG21	14	2.05
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	18	2.05
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	20	2.05
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	14	2.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	6	2.04
(1,1352)	1:82:A:LYS:HA	1:74:A:TYR:HE1	15	2.04
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD23	18	2.04
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD23	20	2.04
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	13	2.04
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG11	12	2.04
(1,1027)	1:59:A:VAL:HG12	1:64:A:TYR:HB2	10	2.04
(1,1005)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	17	2.04
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG23	9	2.04
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG23	18	2.04
(1,867)	1:55:A:THR:HG22	1:54:A:GLY:HA2	10	2.04
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	3	2.04
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	16	2.04
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	3	2.04
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	8	2.04
(1,1859)	1:83:A:TYR:H	1:74:A:TYR:HE1	15	2.03
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	15	2.03
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	12	2.03
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	16	2.03
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	12	2.03
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	8	2.03
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	15	2.03
(1,1028)	1:59:A:VAL:HG13	1:64:A:TYR:HB3	3	2.03
(1,1027)	1:59:A:VAL:HG11	1:64:A:TYR:HB2	2	2.03
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG23	4	2.03
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG22	6	2.03
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	15	2.03
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	19	2.03
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	11	2.03
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	7	2.03
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	19	2.03
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	2	2.03
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	12	2.02
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG23	3	2.02
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	16	2.02
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	9	2.02
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	8	2.02
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	9	2.02
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	12	2.02
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	14	2.02
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	17	2.02
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	19	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1027)	1:59:A:VAL:HG13	1:64:A:TYR:HB2	12	2.02
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG22	16	2.02
(1,943)	1:59:A:VAL:HG11	1:65:A:TYR:HB3	14	2.02
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG23	7	2.02
(1,867)	1:55:A:THR:HG21	1:54:A:GLY:HA2	17	2.02
(1,867)	1:55:A:THR:HG22	1:54:A:GLY:HA2	20	2.02
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG21	14	2.02
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	18	2.02
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	8	2.02
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	5	2.01
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	3	2.01
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	20	2.01
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	19	2.01
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	7	2.01
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD23	1	2.01
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	1	2.01
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	16	2.01
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	20	2.01
(1,962)	1:59:A:VAL:HG23	1:65:A:TYR:H	13	2.01
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG22	5	2.01
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG22	13	2.01
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG21	17	2.01
(1,867)	1:55:A:THR:HG23	1:54:A:GLY:HA2	1	2.01
(1,867)	1:55:A:THR:HG22	1:54:A:GLY:HA2	2	2.01
(1,867)	1:55:A:THR:HG23	1:54:A:GLY:HA2	18	2.01
(1,697)	1:44:A:ALA:HB2	1:34:A:GLY:HA2	19	2.01
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	11	2.01
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	5	2.01
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	14	2.0
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD22	15	2.0
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	8	2.0
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	3	2.0
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	5	2.0
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	11	2.0
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG22	8	2.0
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG21	1	2.0
(1,867)	1:55:A:THR:HG21	1:54:A:GLY:HA2	14	2.0
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD21	18	2.0
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	1	2.0
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	6	2.0
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	10	2.0
(1,18)	1:59:A:VAL:HG11	1:60:A:TYR:HB2	17	2.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	19	1.99
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	4	1.99
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	4	1.99
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	10	1.99
(1,962)	1:59:A:VAL:HG23	1:65:A:TYR:H	5	1.99
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG21	19	1.99
(1,867)	1:55:A:THR:HG23	1:54:A:GLY:HA2	4	1.99
(1,18)	1:59:A:VAL:HG12	1:60:A:TYR:HB2	3	1.99
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	14	1.99
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	9	1.98
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	16	1.98
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	2	1.98
(1,1005)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	16	1.98
(1,965)	1:59:A:VAL:HG22	1:64:A:TYR:H	11	1.98
(1,962)	1:59:A:VAL:HG23	1:65:A:TYR:H	2	1.98
(1,962)	1:59:A:VAL:HG22	1:65:A:TYR:H	8	1.98
(1,948)	1:59:A:VAL:HG12	1:64:A:TYR:HA	17	1.98
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG21	8	1.98
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD22	11	1.98
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	7	1.98
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	7	1.98
(1,239)	1:13:A:CYS:HA	1:14:A:ARG:HG2	2	1.98
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	10	1.98
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	9	1.98
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	6	1.97
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	17	1.97
(1,1506)	1:4:A:TYR:H	1:2:A:VAL:HG23	2	1.97
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD23	17	1.97
(1,1267)	1:79:A:GLN:HA	1:80:A:LEU:HD21	4	1.97
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	5	1.97
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	14	1.97
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	7	1.97
(1,1105)	1:69:A:CYS:HB3	1:68:A:SER:HA	18	1.97
(1,1005)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	2	1.97
(1,962)	1:59:A:VAL:HG22	1:65:A:TYR:H	17	1.97
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG22	13	1.97
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG22	2	1.97
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG22	3	1.97
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG21	16	1.97
(1,867)	1:55:A:THR:HG23	1:54:A:GLY:HA2	8	1.97
(1,867)	1:55:A:THR:HG22	1:54:A:GLY:HA2	16	1.97
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	9	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG23	8	1.97
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	9	1.97
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	14	1.97
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	8	1.97
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	2	1.96
(1,1506)	1:4:A:TYR:H	1:2:A:VAL:HG21	19	1.96
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	19	1.96
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	17	1.96
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	18	1.96
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	17	1.96
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	10	1.96
(1,1028)	1:59:A:VAL:HG13	1:64:A:TYR:HB3	4	1.96
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD22	2	1.96
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD21	5	1.96
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD23	8	1.96
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD22	10	1.96
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD23	16	1.96
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD21	17	1.96
(1,694)	1:44:A:ALA:HB2	1:59:A:VAL:HG11	1	1.96
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	8	1.96
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	8	1.96
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	3	1.96
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	11	1.95
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	9	1.95
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	19	1.95
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	17	1.95
(1,1027)	1:59:A:VAL:HG13	1:64:A:TYR:HB2	19	1.95
(1,1027)	1:59:A:VAL:HG13	1:64:A:TYR:HB2	20	1.95
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG11	18	1.95
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	1	1.95
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD22	7	1.95
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD23	9	1.95
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD23	14	1.95
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD22	19	1.95
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	11	1.95
(1,599)	1:36:A:THR:HG22	1:64:A:TYR:HB3	16	1.95
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	10	1.95
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	6	1.95
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	12	1.95
(1,18)	1:59:A:VAL:HG11	1:60:A:TYR:HB2	5	1.95
(1,18)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	6	1.95
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	16	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	13	1.94
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	4	1.94
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	6	1.94
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	6	1.94
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG12	6	1.94
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG21	17	1.94
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG21	11	1.94
(1,867)	1:55:A:THR:HG21	1:54:A:GLY:HA2	3	1.94
(1,867)	1:55:A:THR:HG21	1:54:A:GLY:HA2	12	1.94
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD21	1	1.94
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD21	4	1.94
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD23	12	1.94
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD22	13	1.94
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD23	15	1.94
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	9	1.94
(1,1602)	1:29:A:CYS:H	1:28:A:LYS:HD2	2	1.93
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	5	1.93
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	12	1.93
(1,1028)	1:59:A:VAL:HG13	1:64:A:TYR:HB3	19	1.93
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG11	17	1.93
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG23	14	1.93
(1,902)	1:58:A:TYR:HA	1:59:A:VAL:HG22	15	1.93
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD23	3	1.93
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	16	1.93
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	14	1.92
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	17	1.92
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	18	1.92
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG13	17	1.92
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	10	1.92
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD21	6	1.92
(1,825)	1:52:A:ASN:H	1:51:A:LEU:HD23	20	1.92
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	13	1.92
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	14	1.92
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	7	1.92
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	9	1.92
(1,18)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	7	1.92
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	1	1.91
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	3	1.91
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	3	1.91
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	10	1.91
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	15	1.91
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	12	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	17	1.91
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	16	1.91
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	17	1.91
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	9	1.91
(1,18)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	8	1.91
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	13	1.9
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG22	19	1.9
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	18	1.9
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD23	1	1.9
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD22	5	1.9
(1,1027)	1:59:A:VAL:HG13	1:64:A:TYR:HB2	3	1.9
(1,962)	1:59:A:VAL:HG21	1:65:A:TYR:H	7	1.9
(1,867)	1:55:A:THR:HG22	1:54:A:GLY:HA2	9	1.9
(1,867)	1:55:A:THR:HG21	1:54:A:GLY:HA2	15	1.9
(1,694)	1:44:A:ALA:HB2	1:59:A:VAL:HG13	12	1.9
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	3	1.9
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	6	1.9
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	7	1.9
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	1	1.9
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	17	1.9
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	1	1.9
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	4	1.89
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	19	1.89
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	8	1.89
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	15	1.89
(1,1027)	1:59:A:VAL:HG13	1:64:A:TYR:HB2	4	1.89
(1,559)	1:33:A:LYS:HG2	1:34:A:GLY:HA3	11	1.89
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG22	5	1.88
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	18	1.88
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	2	1.88
(1,697)	1:44:A:ALA:HB3	1:34:A:GLY:HA2	10	1.88
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	14	1.88
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	1	1.88
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	19	1.88
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	19	1.88
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	6	1.88
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	15	1.88
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	14	1.88
(1,18)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	12	1.88
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	12	1.88
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	4	1.87
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD13	5	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	10	1.87
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	7	1.87
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD23	20	1.87
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG23	15	1.87
(1,867)	1:55:A:THR:HG23	1:54:A:GLY:HA2	6	1.87
(1,867)	1:55:A:THR:HG23	1:54:A:GLY:HA2	19	1.87
(1,694)	1:44:A:ALA:HB3	1:59:A:VAL:HG11	2	1.87
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	17	1.87
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	4	1.87
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	20	1.87
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	18	1.87
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	13	1.87
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD23	7	1.87
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	6	1.87
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	6	1.87
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	17	1.87
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	2	1.87
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD12	18	1.86
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	12	1.86
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD22	19	1.86
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG13	2	1.86
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG13	16	1.86
(1,962)	1:59:A:VAL:HG22	1:65:A:TYR:H	12	1.86
(1,867)	1:55:A:THR:HG22	1:54:A:GLY:HA2	13	1.86
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	12	1.86
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	3	1.85
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	19	1.85
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	20	1.85
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	13	1.85
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	5	1.85
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	18	1.85
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	10	1.85
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	15	1.85
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	19	1.85
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	12	1.85
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG22	17	1.85
(1,945)	1:58:A:TYR:HB2	1:59:A:VAL:HG11	9	1.85
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	4	1.85
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	14	1.85
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	13	1.85
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	10	1.85
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	10	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	8	1.85
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	20	1.85
(1,18)	1:59:A:VAL:HG13	1:60:A:TYR:HB2	2	1.85
(1,18)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	19	1.85
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	10	1.85
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	8	1.84
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	9	1.84
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	1	1.84
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	14	1.84
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	1	1.84
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	2	1.84
(1,1185)	1:72:A:GLY:HA3	1:71:A:TYR:HD1	1	1.84
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	16	1.84
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG22	3	1.84
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	15	1.84
(1,697)	1:44:A:ALA:HB1	1:34:A:GLY:HA2	7	1.84
(1,697)	1:44:A:ALA:HB3	1:34:A:GLY:HA2	12	1.84
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	16	1.84
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	5	1.84
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	2	1.84
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	17	1.84
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	11	1.84
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	7	1.83
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	5	1.83
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG22	16	1.83
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	15	1.83
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	19	1.83
(1,943)	1:59:A:VAL:HG11	1:65:A:TYR:HB3	11	1.83
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	14	1.83
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	8	1.83
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	10	1.83
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	6	1.83
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	10	1.83
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	15	1.83
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	18	1.83
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	14	1.83
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	3	1.83
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	17	1.83
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG21	20	1.83
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	17	1.83
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	7	1.82
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG22	1	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	8	1.82
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	12	1.82
(1,1071)	1:67:A:CYS:HA	1:50:A:CYS:HB3	8	1.82
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG11	19	1.82
(1,948)	1:59:A:VAL:HG12	1:64:A:TYR:HA	7	1.82
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG21	8	1.82
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	1	1.82
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	3	1.82
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	11	1.82
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	1	1.82
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	3	1.82
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	13	1.82
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	1	1.82
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	13	1.82
(1,18)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	4	1.82
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	18	1.81
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	12	1.81
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	3	1.81
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	14	1.81
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	16	1.81
(1,1064)	1:66:A:LYS:HG3	1:59:A:VAL:HG21	6	1.81
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	4	1.81
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	8	1.81
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	9	1.81
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	19	1.81
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	2	1.81
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	15	1.81
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	11	1.81
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	6	1.81
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	5	1.81
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	10	1.81
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	12	1.81
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	1	1.8
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	8	1.8
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	1	1.8
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	2	1.8
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	4	1.8
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	12	1.8
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	17	1.8
(1,1071)	1:67:A:CYS:HA	1:50:A:CYS:HB3	4	1.8
(1,1071)	1:67:A:CYS:HA	1:50:A:CYS:HB3	11	1.8
(1,1071)	1:67:A:CYS:HA	1:50:A:CYS:HB3	14	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG23	13	1.8
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	6	1.8
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG21	19	1.8
(1,43)	1:2:A:VAL:HG22	1:4:A:TYR:HD1	2	1.8
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	2	1.79
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD13	8	1.79
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD12	9	1.79
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	9	1.79
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	13	1.79
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	9	1.79
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	8	1.79
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	13	1.79
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	15	1.79
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	16	1.79
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	18	1.79
(1,962)	1:59:A:VAL:HG21	1:65:A:TYR:H	4	1.79
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG23	4	1.79
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG23	7	1.79
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG21	19	1.79
(1,697)	1:44:A:ALA:HB3	1:34:A:GLY:HA2	1	1.79
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	6	1.79
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	11	1.79
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	6	1.79
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	7	1.79
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	1	1.78
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	9	1.78
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	15	1.78
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	13	1.78
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	19	1.78
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG23	2	1.78
(1,948)	1:59:A:VAL:HG13	1:64:A:TYR:HA	15	1.78
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG21	12	1.78
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	2	1.78
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	1	1.78
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	3	1.78
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	7	1.78
(1,18)	1:59:A:VAL:HG12	1:60:A:TYR:HB2	15	1.78
(1,1539)	1:17:A:GLY:H	1:32:A:ARG:HG2	9	1.77
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD13	3	1.77
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD13	10	1.77
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	17	1.77
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	18	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	3	1.77
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	6	1.77
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG13	11	1.77
(1,599)	1:36:A:THR:HG23	1:64:A:TYR:HB3	2	1.77
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG21	3	1.77
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	4	1.77
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	20	1.77
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	13	1.77
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	9	1.77
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG23	8	1.76
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	3	1.76
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD11	11	1.76
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	2	1.76
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	16	1.76
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD21	2	1.76
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	11	1.76
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	4	1.76
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	9	1.76
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	15	1.76
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	16	1.76
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG22	5	1.76
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	4	1.76
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	19	1.76
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	16	1.76
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD13	1	1.75
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	7	1.75
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	5	1.75
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	14	1.75
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	16	1.75
(1,1071)	1:67:A:CYS:HA	1:50:A:CYS:HB3	15	1.75
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG23	9	1.75
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	3	1.75
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	13	1.75
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	13	1.75
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	20	1.75
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	5	1.75
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	15	1.75
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	3	1.75
(1,18)	1:59:A:VAL:HG13	1:63:A:PRO:HD2	1	1.75
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG21	20	1.74
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD11	4	1.74
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD13	6	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD12	16	1.74
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	12	1.74
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	18	1.74
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	1	1.74
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	9	1.74
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	10	1.74
(1,1071)	1:67:A:CYS:HA	1:50:A:CYS:HB3	16	1.74
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG22	6	1.74
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG21	11	1.74
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	3	1.74
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	13	1.74
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	15	1.74
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	19	1.74
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	8	1.74
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	18	1.74
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	13	1.74
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	3	1.74
(1,23)	1:78:A:CYS:HB2	1:70:A:PRO:HD3	15	1.74
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	10	1.73
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	11	1.73
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	13	1.73
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG23	7	1.73
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD13	14	1.73
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	7	1.73
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	11	1.73
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	12	1.73
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	4	1.73
(1,953)	1:59:A:VAL:HG13	1:60:A:TYR:HD1	9	1.73
(1,952)	1:59:A:VAL:HG13	1:58:A:TYR:HD1	13	1.73
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG21	1	1.73
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG22	10	1.73
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	19	1.73
(1,706)	1:44:A:ALA:HB1	1:64:A:TYR:HD1	3	1.73
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	1	1.73
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	7	1.73
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	5	1.73
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	20	1.73
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	10	1.73
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	3	1.73
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	6	1.73
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	2	1.72
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	16	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	16	1.72
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD12	13	1.72
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD11	19	1.72
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	10	1.72
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	17	1.72
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	20	1.72
(1,1005)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	13	1.72
(1,962)	1:59:A:VAL:HG23	1:65:A:TYR:H	10	1.72
(1,706)	1:44:A:ALA:HB3	1:64:A:TYR:HD1	19	1.72
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	20	1.72
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	17	1.72
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	8	1.72
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	11	1.72
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	18	1.72
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	12	1.71
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	3	1.71
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD12	17	1.71
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	1	1.71
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG12	13	1.71
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG22	2	1.71
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	19	1.71
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	14	1.71
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	5	1.71
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	15	1.71
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	9	1.71
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	12	1.7
(1,1775)	1:65:A:TYR:H	1:63:A:PRO:HB3	20	1.7
(1,1602)	1:29:A:CYS:H	1:28:A:LYS:HD2	12	1.7
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	1	1.7
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	6	1.7
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	20	1.7
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD12	7	1.7
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	2	1.7
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	11	1.7
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	20	1.7
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	14	1.7
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	20	1.7
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	13	1.7
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	7	1.7
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG23	1	1.7
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	6	1.7
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	11	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	17	1.7
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	12	1.7
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	4	1.7
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	7	1.69
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	12	1.69
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	1	1.69
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	9	1.69
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	4	1.69
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	13	1.69
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	14	1.69
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	10	1.69
(1,1185)	1:72:A:GLY:HA3	1:71:A:TYR:HD1	8	1.69
(1,1155)	1:69:A:CYS:HB2	1:70:A:PRO:HG2	3	1.69
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	6	1.69
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	14	1.69
(1,965)	1:59:A:VAL:HG22	1:64:A:TYR:H	16	1.69
(1,939)	1:59:A:VAL:HG13	1:66:A:LYS:HG3	6	1.69
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG22	15	1.69
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG23	18	1.69
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	17	1.69
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	19	1.69
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	13	1.69
(1,18)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	18	1.69
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	5	1.68
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	11	1.68
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	17	1.68
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD13	2	1.68
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD11	20	1.68
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	5	1.68
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	4	1.68
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	5	1.68
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	10	1.68
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD21	12	1.68
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG23	3	1.68
(1,962)	1:59:A:VAL:HG23	1:65:A:TYR:H	6	1.68
(1,962)	1:59:A:VAL:HG22	1:65:A:TYR:H	19	1.68
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	9	1.68
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	3	1.68
(1,697)	1:44:A:ALA:HB2	1:34:A:GLY:HA2	4	1.68
(1,560)	1:34:A:GLY:HA2	1:33:A:LYS:HG2	11	1.68
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	13	1.68
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	13	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:34:A:GLY:HA3	1:58:A:TYR:HB3	12	1.68
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	4	1.67
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	9	1.67
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	10	1.67
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	14	1.67
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	18	1.67
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	10	1.67
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	15	1.67
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	2	1.67
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	6	1.67
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	17	1.67
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	3	1.67
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	9	1.67
(1,1273)	1:79:A:GLN:HB3	1:80:A:LEU:HD22	15	1.67
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	3	1.67
(1,1071)	1:67:A:CYS:HA	1:50:A:CYS:HB3	10	1.67
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	9	1.67
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	7	1.67
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	17	1.67
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	9	1.67
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	16	1.67
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	12	1.67
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	7	1.67
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	7	1.67
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	20	1.67
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	2	1.67
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	17	1.67
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	8	1.67
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	16	1.67
(1,1857)	1:83:A:TYR:H	1:82:A:LYS:HG2	6	1.66
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	2	1.66
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	8	1.66
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	13	1.66
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	18	1.66
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD12	12	1.66
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	3	1.66
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	17	1.66
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	4	1.66
(1,1278)	1:79:A:GLN:HB2	1:78:A:CYS:H	9	1.66
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	6	1.66
(1,1028)	1:59:A:VAL:HG11	1:64:A:TYR:HB3	1	1.66
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	20	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	1	1.66
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	2	1.66
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	10	1.66
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	3	1.66
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	1	1.66
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	4	1.66
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	7	1.66
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	20	1.65
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG22	10	1.65
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	13	1.65
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	16	1.65
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	19	1.65
(1,1228)	1:75:A:GLY:HA3	1:76:A:LYS:HG3	7	1.65
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG12	9	1.65
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	11	1.65
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG11	14	1.65
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	2	1.65
(1,869)	1:55:A:THR:HG22	1:68:A:SER:HB3	6	1.65
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD23	14	1.65
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	1	1.65
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	19	1.65
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	16	1.65
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	15	1.64
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	6	1.64
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	14	1.64
(1,1394)	1:82:A:LYS:HA	1:81:A:LYS:HB2	8	1.64
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	7	1.64
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	9	1.64
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	18	1.64
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	13	1.64
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	9	1.64
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	12	1.64
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	9	1.64
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG21	17	1.64
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	2	1.64
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	1	1.64
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	10	1.64
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	9	1.64
(1,1427)	1:52:A:ASN:HA	1:51:A:LEU:HD12	15	1.63
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	20	1.63
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	5	1.63
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	19	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	18	1.63
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	11	1.63
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	3	1.63
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG21	7	1.63
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	9	1.63
(1,706)	1:44:A:ALA:HB1	1:64:A:TYR:HD1	20	1.63
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	6	1.63
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG21	3	1.63
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	11	1.63
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	3	1.63
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	2	1.63
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	15	1.62
(1,1498)	1:46:A:PHE:HA	1:47:A:PRO:HA	19	1.62
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG21	17	1.62
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	18	1.62
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	16	1.62
(1,1005)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	5	1.62
(1,965)	1:59:A:VAL:HG22	1:64:A:TYR:H	17	1.62
(1,948)	1:59:A:VAL:HG11	1:64:A:TYR:HA	2	1.62
(1,943)	1:59:A:VAL:HG13	1:65:A:TYR:HB3	13	1.62
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	9	1.62
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	3	1.62
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	15	1.62
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	4	1.62
(1,576)	1:73:A:TYR:HA	1:70:A:PRO:HB3	9	1.62
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	17	1.62
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	16	1.62
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	1	1.62
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	5	1.62
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	18	1.62
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	10	1.62
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	13	1.62
(1,18)	1:59:A:VAL:HG13	1:60:A:TYR:HB2	11	1.62
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	17	1.61
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	19	1.61
(1,1228)	1:75:A:GLY:HA3	1:76:A:LYS:HG3	4	1.61
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	7	1.61
(1,1027)	1:59:A:VAL:HG11	1:64:A:TYR:HB2	1	1.61
(1,1005)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	15	1.61
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	12	1.61
(1,965)	1:59:A:VAL:HG23	1:64:A:TYR:H	5	1.61
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG11	11	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	1	1.61
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	11	1.61
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	20	1.61
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	9	1.61
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	20	1.61
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	4	1.61
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	6	1.61
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	19	1.61
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	16	1.61
(1,18)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	10	1.61
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	16	1.6
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	20	1.6
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	4	1.6
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	1	1.6
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	6	1.6
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	3	1.6
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG21	4	1.6
(1,1005)	1:59:A:VAL:HG13	1:63:A:PRO:HD2	3	1.6
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	2	1.6
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	3	1.6
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	6	1.6
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	7	1.6
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	18	1.6
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	19	1.6
(1,943)	1:59:A:VAL:HG11	1:65:A:TYR:HB3	16	1.6
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	2	1.6
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	8	1.6
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	9	1.6
(1,641)	1:39:A:ASN:HA	1:29:A:CYS:HB3	5	1.6
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	8	1.6
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	3	1.6
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	4	1.6
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	16	1.6
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	18	1.6
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	2	1.59
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	14	1.59
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	6	1.59
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	19	1.59
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	5	1.59
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	8	1.59
(1,1185)	1:72:A:GLY:HA3	1:71:A:TYR:HD1	17	1.59
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	13	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	18	1.59
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG12	3	1.59
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	16	1.59
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	17	1.59
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	19	1.59
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	19	1.59
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	3	1.59
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	17	1.59
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	14	1.59
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	2	1.59
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	3	1.59
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	8	1.59
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	10	1.59
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	10	1.59
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	18	1.59
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	5	1.58
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	9	1.58
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	5	1.58
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	9	1.58
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	1	1.58
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	6	1.58
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG21	18	1.58
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	4	1.58
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	9	1.58
(1,943)	1:59:A:VAL:HG13	1:65:A:TYR:HB3	15	1.58
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	2	1.58
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	20	1.58
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	5	1.58
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	9	1.58
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	9	1.58
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	5	1.58
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	18	1.58
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	20	1.58
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG21	13	1.57
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	3	1.57
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	8	1.57
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	11	1.57
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	17	1.57
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	19	1.57
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD23	13	1.57
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD23	17	1.57
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG22	12	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	20	1.57
(1,948)	1:59:A:VAL:HG11	1:64:A:TYR:HA	10	1.57
(1,948)	1:59:A:VAL:HG12	1:64:A:TYR:HA	18	1.57
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG21	16	1.57
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	12	1.57
(1,521)	1:32:A:ARG:HB3	1:31:A:CYS:HA	2	1.57
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	4	1.57
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	11	1.57
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	6	1.56
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	13	1.56
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	4	1.56
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	12	1.56
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	6	1.56
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	17	1.56
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	1	1.56
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	20	1.56
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	15	1.56
(1,940)	1:59:A:VAL:HG12	1:66:A:LYS:HG2	1	1.56
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	17	1.56
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	2	1.56
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	20	1.56
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	5	1.56
(1,694)	1:44:A:ALA:HB2	1:59:A:VAL:HG11	9	1.56
(1,306)	1:18:A:THR:HG21	1:20:A:LYS:HA	10	1.56
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	8	1.55
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	11	1.55
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	13	1.55
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	4	1.55
(1,1228)	1:75:A:GLY:HA3	1:76:A:LYS:HG3	12	1.55
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	1	1.55
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	8	1.55
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	10	1.55
(1,962)	1:59:A:VAL:HG21	1:65:A:TYR:H	18	1.55
(1,952)	1:59:A:VAL:HG12	1:58:A:TYR:HD1	17	1.55
(1,943)	1:59:A:VAL:HG13	1:65:A:TYR:HB3	8	1.55
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	7	1.55
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	18	1.55
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	8	1.55
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	11	1.55
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	12	1.55
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	19	1.55
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	11	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	1	1.55
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	4	1.55
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	7	1.55
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	6	1.55
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	9	1.55
(1,4)	1:7:A:PRO:HA	1:21:A:LYS:HE2	20	1.55
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	2	1.54
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	2	1.54
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	16	1.54
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	3	1.54
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	11	1.54
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG23	10	1.54
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	11	1.54
(1,985)	1:62:A:TYR:HA	1:63:A:PRO:HA	5	1.54
(1,962)	1:59:A:VAL:HG22	1:65:A:TYR:H	1	1.54
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG23	14	1.54
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	13	1.54
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	15	1.54
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	8	1.54
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	18	1.54
(1,706)	1:44:A:ALA:HB2	1:64:A:TYR:HD1	16	1.54
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	20	1.54
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD23	4	1.54
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	9	1.54
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	2	1.54
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	11	1.54
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	13	1.54
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	5	1.54
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	10	1.54
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	20	1.54
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	16	1.54
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	10	1.54
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	20	1.53
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	9	1.53
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	17	1.53
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	6	1.53
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	16	1.53
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	14	1.53
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	12	1.53
(1,953)	1:59:A:VAL:HG11	1:60:A:TYR:HD1	5	1.53
(1,952)	1:59:A:VAL:HG13	1:58:A:TYR:HD1	8	1.53
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	20	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	10	1.53
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	15	1.53
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	18	1.53
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	11	1.53
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	19	1.53
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	10	1.52
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	19	1.52
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	11	1.52
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	15	1.52
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	12	1.52
(1,1345)	1:81:A:LYS:HG3	1:83:A:TYR:H	2	1.52
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD12	7	1.52
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	18	1.52
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	3	1.52
(1,915)	1:58:A:TYR:HB3	1:59:A:VAL:HG22	20	1.52
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	1	1.52
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	15	1.52
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	18	1.52
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	20	1.52
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	19	1.52
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	8	1.52
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	2	1.52
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	9	1.52
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	16	1.52
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	1	1.51
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	13	1.51
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	14	1.51
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	10	1.51
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	20	1.51
(1,1379)	1:82:A:LYS:HE2	1:74:A:TYR:HE1	15	1.51
(1,1228)	1:75:A:GLY:HA3	1:76:A:LYS:HG3	1	1.51
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	19	1.51
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	15	1.51
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG12	17	1.51
(1,943)	1:59:A:VAL:HG12	1:65:A:TYR:HB3	5	1.51
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	2	1.51
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	5	1.51
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	5	1.51
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	8	1.51
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	6	1.51
(1,306)	1:18:A:THR:HG23	1:20:A:LYS:HA	17	1.51
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	15	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:13:A:CYS:HB2	1:11:A:TYR:HD1	13	1.51
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG22	18	1.51
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	13	1.51
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	6	1.51
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	3	1.5
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	7	1.5
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	12	1.5
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	15	1.5
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	1	1.5
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	6	1.5
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD13	9	1.5
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	3	1.5
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	9	1.5
(1,960)	1:59:A:VAL:HG21	1:60:A:TYR:HB2	9	1.5
(1,948)	1:59:A:VAL:HG13	1:64:A:TYR:HA	12	1.5
(1,943)	1:59:A:VAL:HG13	1:65:A:TYR:HB3	7	1.5
(1,943)	1:59:A:VAL:HG12	1:65:A:TYR:HB3	17	1.5
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	16	1.5
(1,869)	1:55:A:THR:HG23	1:68:A:SER:HB3	14	1.5
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	16	1.5
(1,697)	1:44:A:ALA:HB3	1:34:A:GLY:HA2	9	1.5
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	14	1.5
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	1	1.5
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	6	1.5
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	11	1.5
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE2	15	1.5
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	7	1.49
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	16	1.49
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG22	6	1.49
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	4	1.49
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	4	1.49
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	11	1.49
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	18	1.49
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	14	1.49
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	15	1.49
(1,965)	1:59:A:VAL:HG23	1:64:A:TYR:H	2	1.49
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	14	1.49
(1,694)	1:44:A:ALA:HB1	1:59:A:VAL:HG12	6	1.49
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	13	1.49
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	18	1.49
(1,166)	1:7:A:PRO:HD3	1:21:A:LYS:HG3	16	1.49
(1,4)	1:7:A:PRO:HA	1:21:A:LYS:HE2	4	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	5	1.49
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG21	15	1.48
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	5	1.48
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	8	1.48
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	9	1.48
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	19	1.48
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	20	1.48
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	7	1.48
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD21	6	1.48
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	4	1.48
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG11	5	1.48
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	2	1.48
(1,965)	1:59:A:VAL:HG22	1:64:A:TYR:H	8	1.48
(1,965)	1:59:A:VAL:HG23	1:64:A:TYR:H	13	1.48
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	4	1.48
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	15	1.48
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	19	1.48
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	10	1.48
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	20	1.48
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	12	1.48
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	20	1.48
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	19	1.48
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	2	1.48
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	9	1.48
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	16	1.48
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	8	1.48
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	9	1.48
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	11	1.48
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	3	1.48
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	20	1.48
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	6	1.48
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	14	1.47
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG21	12	1.47
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	16	1.47
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	11	1.47
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	16	1.47
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	7	1.47
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	2	1.47
(1,1337)	1:81:A:LYS:HB2	1:83:A:TYR:HE1	6	1.47
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD23	18	1.47
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	14	1.47
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	19	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	12	1.47
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	20	1.47
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	8	1.47
(1,1005)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	6	1.47
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	13	1.47
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	6	1.47
(1,869)	1:55:A:THR:HG21	1:68:A:SER:HB3	4	1.47
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	12	1.47
(1,697)	1:44:A:ALA:HB2	1:34:A:GLY:HA2	6	1.47
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	9	1.47
(1,599)	1:36:A:THR:HG22	1:64:A:TYR:HB3	6	1.47
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	14	1.47
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	7	1.47
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	15	1.47
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	6	1.47
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	5	1.47
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	6	1.47
(1,123)	1:5:A:PRO:HB3	1:3:A:TYR:HD1	12	1.47
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	7	1.47
(1,15)	1:40:A:CYS:HB2	1:32:A:ARG:HB3	9	1.47
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	2	1.46
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	11	1.46
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	7	1.46
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	16	1.46
(1,1379)	1:82:A:LYS:HE2	1:74:A:TYR:HE1	6	1.46
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	9	1.46
(1,1185)	1:72:A:GLY:HA3	1:71:A:TYR:HD1	13	1.46
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	5	1.46
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	9	1.46
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	17	1.46
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG13	13	1.46
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	20	1.46
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	10	1.46
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	1	1.46
(1,790)	1:51:A:LEU:HD12	1:51:A:LEU:HA	3	1.46
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	8	1.46
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	18	1.46
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	4	1.46
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	13	1.46
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	12	1.46
(1,183)	1:7:A:PRO:HG3	1:21:A:LYS:HG3	20	1.46
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	3	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:59:A:VAL:HG13	1:63:A:PRO:HD2	9	1.46
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	10	1.45
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	1	1.45
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	12	1.45
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	9	1.45
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD12	2	1.45
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	5	1.45
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	14	1.45
(1,953)	1:59:A:VAL:HG11	1:60:A:TYR:HD1	6	1.45
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	9	1.45
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	20	1.45
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	11	1.45
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	18	1.45
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	7	1.45
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	16	1.45
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	13	1.45
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	18	1.45
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	13	1.45
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	14	1.45
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	19	1.45
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	5	1.45
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	19	1.45
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	17	1.45
(1,306)	1:18:A:THR:HG21	1:20:A:LYS:HA	1	1.45
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	19	1.45
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	17	1.45
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	9	1.45
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	19	1.45
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	15	1.45
(1,1476)	1:30:A:TYR:HB3	1:18:A:THR:HG23	14	1.44
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	4	1.44
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	10	1.44
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	18	1.44
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	1	1.44
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	20	1.44
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	5	1.44
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	4	1.44
(1,1005)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	7	1.44
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	16	1.44
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	10	1.44
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	17	1.44
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	9	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	7	1.44
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	13	1.44
(1,790)	1:51:A:LEU:HD11	1:51:A:LEU:HA	12	1.44
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	18	1.44
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	20	1.44
(1,617)	1:38:A:LYS:HA	1:38:A:LYS:HE3	7	1.44
(1,599)	1:36:A:THR:HG21	1:64:A:TYR:HB3	9	1.44
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	12	1.44
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	14	1.44
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	20	1.44
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	13	1.44
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	19	1.44
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	9	1.44
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	10	1.44
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	16	1.44
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	12	1.44
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	19	1.43
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	17	1.43
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	14	1.43
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	20	1.43
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	17	1.43
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	9	1.43
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	17	1.43
(1,1185)	1:72:A:GLY:HA3	1:71:A:TYR:HD1	16	1.43
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	3	1.43
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	15	1.43
(1,1005)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	8	1.43
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG12	7	1.43
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG12	12	1.43
(1,965)	1:59:A:VAL:HG23	1:64:A:TYR:H	15	1.43
(1,953)	1:59:A:VAL:HG11	1:60:A:TYR:HD1	17	1.43
(1,790)	1:51:A:LEU:HD12	1:51:A:LEU:HA	2	1.43
(1,790)	1:51:A:LEU:HD11	1:51:A:LEU:HA	15	1.43
(1,790)	1:51:A:LEU:HD13	1:51:A:LEU:HA	19	1.43
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	20	1.43
(1,697)	1:44:A:ALA:HB2	1:34:A:GLY:HA2	11	1.43
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	12	1.43
(1,564)	1:34:A:GLY:HA3	1:58:A:TYR:HE1	20	1.43
(1,560)	1:34:A:GLY:HA2	1:33:A:LYS:HG2	20	1.43
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD21	11	1.43
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	20	1.43
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	12	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	3	1.43
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	3	1.43
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	15	1.43
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	18	1.43
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	20	1.43
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	2	1.43
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	5	1.43
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	5	1.43
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	9	1.42
(1,1458)	1:29:A:CYS:HA	1:30:A:TYR:HB3	6	1.42
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD12	2	1.42
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	19	1.42
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	4	1.42
(1,952)	1:59:A:VAL:HG12	1:58:A:TYR:HD1	10	1.42
(1,943)	1:59:A:VAL:HG13	1:65:A:TYR:HB3	19	1.42
(1,943)	1:59:A:VAL:HG11	1:65:A:TYR:HB3	20	1.42
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	9	1.42
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	11	1.42
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	19	1.42
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	13	1.42
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	10	1.42
(1,790)	1:51:A:LEU:HD11	1:51:A:LEU:HA	7	1.42
(1,790)	1:51:A:LEU:HD11	1:51:A:LEU:HA	13	1.42
(1,790)	1:51:A:LEU:HD13	1:51:A:LEU:HA	20	1.42
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	15	1.42
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	20	1.42
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	19	1.42
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	1	1.42
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	7	1.42
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	18	1.42
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	16	1.42
(1,497)	1:67:A:CYS:HB2	1:50:A:CYS:HB3	14	1.42
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG22	14	1.42
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	14	1.42
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	7	1.42
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	7	1.41
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	18	1.41
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	7	1.41
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	20	1.41
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	13	1.41
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	10	1.41
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	12	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	14	1.41
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	10	1.41
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	18	1.41
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	8	1.41
(1,965)	1:59:A:VAL:HG23	1:64:A:TYR:H	3	1.41
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	7	1.41
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	17	1.41
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	12	1.41
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	18	1.41
(1,790)	1:51:A:LEU:HD12	1:51:A:LEU:HA	1	1.41
(1,790)	1:51:A:LEU:HD11	1:51:A:LEU:HA	16	1.41
(1,790)	1:51:A:LEU:HD11	1:51:A:LEU:HA	18	1.41
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	14	1.41
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	6	1.41
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	19	1.41
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	10	1.41
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	15	1.41
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	16	1.41
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	19	1.41
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	2	1.4
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	9	1.4
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	19	1.4
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD12	13	1.4
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	18	1.4
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG21	13	1.4
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	12	1.4
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	8	1.4
(1,1005)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	12	1.4
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	9	1.4
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	7	1.4
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	8	1.4
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	20	1.4
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	9	1.4
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	17	1.4
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	3	1.4
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	17	1.4
(1,790)	1:51:A:LEU:HD13	1:51:A:LEU:HA	4	1.4
(1,790)	1:51:A:LEU:HD13	1:51:A:LEU:HA	11	1.4
(1,703)	1:44:A:ALA:HB3	1:58:A:TYR:HA	10	1.4
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	4	1.4
(1,497)	1:67:A:CYS:HB2	1:50:A:CYS:HB3	11	1.4
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	1	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	1	1.4
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	2	1.4
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	5	1.4
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	6	1.4
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	8	1.4
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	12	1.4
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	13	1.4
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	17	1.4
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	1	1.4
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	4	1.4
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	20	1.4
(1,23)	1:78:A:CYS:HB2	1:70:A:PRO:HD3	20	1.4
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	9	1.4
(1,1645)	1:35:A:TYR:H	1:33:A:LYS:HG2	8	1.39
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	9	1.39
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	12	1.39
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	7	1.39
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	12	1.39
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	5	1.39
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD13	7	1.39
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD12	11	1.39
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	19	1.39
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	6	1.39
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	20	1.39
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	5	1.39
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG22	19	1.39
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	3	1.39
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	4	1.39
(1,948)	1:59:A:VAL:HG13	1:64:A:TYR:HA	3	1.39
(1,948)	1:59:A:VAL:HG13	1:64:A:TYR:HA	4	1.39
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	13	1.39
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	1	1.39
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	18	1.39
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	7	1.39
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	15	1.39
(1,790)	1:51:A:LEU:HD12	1:51:A:LEU:HA	5	1.39
(1,790)	1:51:A:LEU:HD12	1:51:A:LEU:HA	10	1.39
(1,790)	1:51:A:LEU:HD11	1:51:A:LEU:HA	17	1.39
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	18	1.39
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	14	1.39
(1,306)	1:18:A:THR:HG22	1:20:A:LYS:HA	2	1.39
(1,306)	1:18:A:THR:HG22	1:20:A:LYS:HA	7	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:18:A:THR:HG22	1:20:A:LYS:HA	14	1.39
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	6	1.39
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	11	1.39
(1,183)	1:7:A:PRO:HG3	1:21:A:LYS:HG3	7	1.39
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	11	1.39
(1,18)	1:59:A:VAL:HG13	1:63:A:PRO:HD2	20	1.39
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	17	1.39
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	9	1.38
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	6	1.38
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD13	20	1.38
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD13	10	1.38
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	15	1.38
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	6	1.38
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	18	1.38
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	6	1.38
(1,962)	1:59:A:VAL:HG23	1:65:A:TYR:H	20	1.38
(1,918)	1:57:A:GLY:HA2	1:58:A:TYR:HB3	13	1.38
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	6	1.38
(1,790)	1:51:A:LEU:HD12	1:51:A:LEU:HA	6	1.38
(1,790)	1:51:A:LEU:HD12	1:51:A:LEU:HA	8	1.38
(1,790)	1:51:A:LEU:HD11	1:51:A:LEU:HA	9	1.38
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	16	1.38
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	16	1.38
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	18	1.38
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	17	1.38
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG23	1	1.38
(1,306)	1:18:A:THR:HG21	1:20:A:LYS:HA	5	1.38
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	3	1.38
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	9	1.38
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	10	1.38
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	7	1.38
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	13	1.38
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	2	1.37
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	13	1.37
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	8	1.37
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	7	1.37
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	2	1.37
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	11	1.37
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	14	1.37
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	16	1.37
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	3	1.37
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	1	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	11	1.37
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	14	1.37
(1,1174)	1:72:A:GLY:HA3	1:82:A:LYS:HG2	20	1.37
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	12	1.37
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	19	1.37
(1,1005)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	19	1.37
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG11	6	1.37
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	18	1.37
(1,953)	1:59:A:VAL:HG12	1:60:A:TYR:HD1	12	1.37
(1,943)	1:59:A:VAL:HG13	1:65:A:TYR:HB3	3	1.37
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	12	1.37
(1,869)	1:55:A:THR:HG23	1:68:A:SER:HB3	3	1.37
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	2	1.37
(1,790)	1:51:A:LEU:HD12	1:51:A:LEU:HA	14	1.37
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG21	17	1.37
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG22	14	1.37
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	11	1.37
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	16	1.37
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	20	1.37
(1,306)	1:18:A:THR:HG22	1:20:A:LYS:HA	8	1.37
(1,306)	1:18:A:THR:HG23	1:20:A:LYS:HA	13	1.37
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	20	1.37
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	1	1.37
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	17	1.37
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	16	1.37
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	4	1.37
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	14	1.37
(1,166)	1:7:A:PRO:HD3	1:21:A:LYS:HG3	7	1.37
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	8	1.37
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	4	1.36
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	3	1.36
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	12	1.36
(1,1347)	1:82:A:LYS:HA	1:82:A:LYS:HG2	6	1.36
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	1	1.36
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD13	3	1.36
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	12	1.36
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	18	1.36
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	3	1.36
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	5	1.36
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	15	1.36
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	17	1.36
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	13	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	15	1.36
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	11	1.36
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	17	1.36
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	20	1.36
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG12	19	1.36
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	5	1.36
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	18	1.36
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	19	1.36
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	18	1.36
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	2	1.36
(1,530)	1:32:A:ARG:HA	1:32:A:ARG:HD2	9	1.36
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	6	1.36
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	5	1.36
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG23	11	1.36
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG23	19	1.36
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	11	1.36
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	5	1.36
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	11	1.36
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	7	1.36
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	5	1.35
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	2	1.35
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	11	1.35
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	2	1.35
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	7	1.35
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	13	1.35
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	16	1.35
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	13	1.35
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	1	1.35
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	9	1.35
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	6	1.35
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	6	1.35
(1,948)	1:59:A:VAL:HG13	1:64:A:TYR:HA	20	1.35
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	1	1.35
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	6	1.35
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	17	1.35
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	1	1.35
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	3	1.35
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	8	1.35
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	8	1.35
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	17	1.35
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	13	1.35
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	3	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	18	1.35
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	19	1.35
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	20	1.35
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG21	20	1.35
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	10	1.35
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	18	1.35
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	8	1.34
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	1	1.34
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD21	9	1.34
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	18	1.34
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD12	4	1.34
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD12	15	1.34
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	1	1.34
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	14	1.34
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	18	1.34
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	8	1.34
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	8	1.34
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	10	1.34
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	12	1.34
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	18	1.34
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	20	1.34
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	2	1.34
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	1	1.34
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	7	1.34
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	3	1.34
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	12	1.34
(1,1005)	1:59:A:VAL:HG12	1:63:A:PRO:HD2	4	1.34
(1,953)	1:59:A:VAL:HG12	1:60:A:TYR:HD1	7	1.34
(1,952)	1:59:A:VAL:HG13	1:58:A:TYR:HD1	7	1.34
(1,952)	1:59:A:VAL:HG13	1:58:A:TYR:HD1	12	1.34
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	18	1.34
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	2	1.34
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	4	1.34
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	19	1.34
(1,869)	1:55:A:THR:HG22	1:68:A:SER:HB3	8	1.34
(1,706)	1:44:A:ALA:HB3	1:64:A:TYR:HD1	15	1.34
(1,614)	1:38:A:LYS:HA	1:38:A:LYS:HG2	13	1.34
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	13	1.34
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	11	1.34
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	10	1.34
(1,455)	1:27:A:TYR:HA	1:21:A:LYS:HB2	11	1.34
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	7	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	14	1.34
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	7	1.34
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	7	1.34
(1,211)	1:10:A:PRO:HA	1:9:A:SER:HA	11	1.34
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	6	1.34
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	13	1.34
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	18	1.34
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	17	1.33
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	6	1.33
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	1	1.33
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	5	1.33
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	7	1.33
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	6	1.33
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	8	1.33
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	15	1.33
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	7	1.33
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	12	1.33
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG12	5	1.33
(1,943)	1:59:A:VAL:HG11	1:65:A:TYR:HB3	2	1.33
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	3	1.33
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	4	1.33
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	7	1.33
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	12	1.33
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	17	1.33
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	11	1.33
(1,568)	1:34:A:GLY:HA2	1:58:A:TYR:HE1	14	1.33
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	2	1.33
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG23	17	1.33
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	18	1.33
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	19	1.33
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	9	1.33
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	10	1.33
(1,166)	1:7:A:PRO:HD3	1:21:A:LYS:HG3	20	1.33
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	11	1.33
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	11	1.32
(1,1602)	1:29:A:CYS:H	1:28:A:LYS:HD2	11	1.32
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	17	1.32
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	14	1.32
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	6	1.32
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	8	1.32
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	12	1.32
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	4	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:72:A:GLY:HA2	1:73:A:TYR:HB3	9	1.32
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	11	1.32
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	4	1.32
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	7	1.32
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	13	1.32
(1,952)	1:59:A:VAL:HG13	1:58:A:TYR:HD1	3	1.32
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	8	1.32
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	14	1.32
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	16	1.32
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	14	1.32
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	10	1.32
(1,497)	1:67:A:CYS:HB2	1:50:A:CYS:HB3	16	1.32
(1,483)	1:28:A:LYS:HB3	1:28:A:LYS:HE2	17	1.32
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	4	1.32
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	12	1.32
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	13	1.32
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	20	1.32
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	16	1.32
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	18	1.32
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	11	1.32
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	2	1.32
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	8	1.32
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	12	1.31
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	20	1.31
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	1	1.31
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	8	1.31
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	9	1.31
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD13	16	1.31
(1,1028)	1:59:A:VAL:HG11	1:64:A:TYR:HB3	9	1.31
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	10	1.31
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	10	1.31
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	10	1.31
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	2	1.31
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	10	1.31
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	7	1.31
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	13	1.31
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	15	1.31
(1,706)	1:44:A:ALA:HB2	1:64:A:TYR:HD1	7	1.31
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	4	1.31
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	20	1.31
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	7	1.31
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	20	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	16	1.31
(1,306)	1:18:A:THR:HG22	1:20:A:LYS:HA	3	1.31
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	13	1.31
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	11	1.31
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	13	1.31
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	8	1.31
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	11	1.31
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG21	7	1.31
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	9	1.3
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	19	1.3
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	2	1.3
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	11	1.3
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	8	1.3
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	18	1.3
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	13	1.3
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	20	1.3
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	8	1.3
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	1	1.3
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	13	1.3
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG22	1	1.3
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG12	4	1.3
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	19	1.3
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG13	8	1.3
(1,943)	1:59:A:VAL:HG13	1:65:A:TYR:HB3	4	1.3
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	15	1.3
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	8	1.3
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	17	1.3
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	10	1.3
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	16	1.3
(1,869)	1:55:A:THR:HG22	1:68:A:SER:HB3	19	1.3
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	6	1.3
(1,633)	1:66:A:LYS:HE2	1:66:A:LYS:HG3	19	1.3
(1,617)	1:38:A:LYS:HA	1:38:A:LYS:HE3	2	1.3
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	9	1.3
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	4	1.3
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	14	1.3
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	9	1.3
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG22	18	1.3
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	2	1.3
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	9	1.3
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	6	1.3
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	14	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	13	1.3
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	1	1.3
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	13	1.3
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	19	1.3
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	19	1.29
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	9	1.29
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	1	1.29
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	2	1.29
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	4	1.29
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	13	1.29
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	13	1.29
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	19	1.29
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	2	1.29
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	10	1.29
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD22	11	1.29
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD13	15	1.29
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	16	1.29
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	3	1.29
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	4	1.29
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	10	1.29
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	17	1.29
(1,1027)	1:59:A:VAL:HG11	1:64:A:TYR:HB2	9	1.29
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG13	1	1.29
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	14	1.29
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	1	1.29
(1,937)	1:60:A:TYR:H	1:59:A:VAL:HB	11	1.29
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	5	1.29
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	8	1.29
(1,869)	1:55:A:THR:HG23	1:68:A:SER:HB3	17	1.29
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	6	1.29
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	6	1.29
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	9	1.29
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	15	1.29
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	20	1.29
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	4	1.29
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	13	1.29
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	18	1.29
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	16	1.29
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	6	1.29
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	14	1.29
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	3	1.29
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	17	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	1	1.29
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	14	1.29
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	3	1.28
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	5	1.28
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	7	1.28
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	15	1.28
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	2	1.28
(1,1312)	1:80:A:LEU:HA	1:80:A:LEU:HD11	10	1.28
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	15	1.28
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	1	1.28
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	6	1.28
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	13	1.28
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	1	1.28
(1,1064)	1:66:A:LYS:HG3	1:59:A:VAL:HG21	20	1.28
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	3	1.28
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG21	14	1.28
(1,866)	1:55:A:THR:HG21	1:56:A:CYS:HB2	19	1.28
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	16	1.28
(1,706)	1:44:A:ALA:HB2	1:64:A:TYR:HD1	5	1.28
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG21	20	1.28
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	10	1.28
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG21	13	1.28
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	6	1.28
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	6	1.28
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	20	1.28
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	5	1.28
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	15	1.28
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	17	1.28
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	10	1.28
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	14	1.28
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	7	1.28
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	12	1.28
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	11	1.27
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	4	1.27
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	20	1.27
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	18	1.27
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	13	1.27
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	14	1.27
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	14	1.27
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	15	1.27
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	3	1.27
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	4	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	5	1.27
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	18	1.27
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD13	7	1.27
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	18	1.27
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	2	1.27
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	5	1.27
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	3	1.27
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	19	1.27
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	19	1.27
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	9	1.27
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	1	1.27
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	14	1.27
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	5	1.27
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	6	1.27
(1,1005)	1:59:A:VAL:HG13	1:63:A:PRO:HD2	1	1.27
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG12	13	1.27
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG13	16	1.27
(1,953)	1:59:A:VAL:HG12	1:60:A:TYR:HD1	8	1.27
(1,869)	1:55:A:THR:HG23	1:68:A:SER:HB3	10	1.27
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	5	1.27
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	5	1.27
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	16	1.27
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	18	1.27
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG22	9	1.27
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	11	1.27
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	3	1.27
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	2	1.27
(1,340)	1:20:A:LYS:HE3	1:18:A:THR:HG23	14	1.27
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	17	1.27
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	13	1.27
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	14	1.27
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	12	1.27
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	13	1.27
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE3	11	1.27
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	1	1.26
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	2	1.26
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	5	1.26
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	16	1.26
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	10	1.26
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	20	1.26
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	5	1.26
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	3	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	16	1.26
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	7	1.26
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	11	1.26
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	15	1.26
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	18	1.26
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	11	1.26
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	20	1.26
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	4	1.26
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	16	1.26
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG23	6	1.26
(1,965)	1:59:A:VAL:HG22	1:64:A:TYR:H	12	1.26
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG22	11	1.26
(1,953)	1:59:A:VAL:HG12	1:60:A:TYR:HD1	3	1.26
(1,953)	1:59:A:VAL:HG11	1:60:A:TYR:HD1	10	1.26
(1,953)	1:59:A:VAL:HG12	1:60:A:TYR:HD1	13	1.26
(1,952)	1:59:A:VAL:HG13	1:58:A:TYR:HD1	15	1.26
(1,943)	1:59:A:VAL:HG12	1:65:A:TYR:HB3	10	1.26
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	5	1.26
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	3	1.26
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	11	1.26
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	17	1.26
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	3	1.26
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	8	1.26
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	14	1.26
(1,599)	1:36:A:THR:HG22	1:64:A:TYR:HB3	18	1.26
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	18	1.26
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	10	1.26
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG23	8	1.26
(1,307)	1:18:A:THR:HG22	1:30:A:TYR:HE1	11	1.26
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	1	1.26
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	10	1.26
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	14	1.26
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	5	1.26
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	3	1.26
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	10	1.26
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	5	1.26
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	8	1.26
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	7	1.25
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	14	1.25
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	6	1.25
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	11	1.25
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	14	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	16	1.25
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	18	1.25
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	6	1.25
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	7	1.25
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	9	1.25
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	3	1.25
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	8	1.25
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	17	1.25
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	9	1.25
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	13	1.25
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	16	1.25
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	20	1.25
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	6	1.25
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	12	1.25
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	11	1.25
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG21	2	1.25
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG13	20	1.25
(1,965)	1:59:A:VAL:HG21	1:64:A:TYR:H	7	1.25
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG23	15	1.25
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	18	1.25
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	4	1.25
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	2	1.25
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	4	1.25
(1,647)	1:39:A:ASN:HB2	1:41:A:GLN:HB3	13	1.25
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	10	1.25
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	9	1.25
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	16	1.25
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	1	1.25
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	16	1.25
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	6	1.25
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	6	1.25
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	10	1.25
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	8	1.25
(1,306)	1:18:A:THR:HG21	1:20:A:LYS:HA	16	1.25
(1,306)	1:18:A:THR:HG21	1:20:A:LYS:HA	19	1.25
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	1	1.25
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	17	1.25
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	6	1.25
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	1	1.25
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	12	1.25
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	16	1.25
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	18	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	13	1.25
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	13	1.24
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	8	1.24
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	10	1.24
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	13	1.24
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	11	1.24
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	15	1.24
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	13	1.24
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	16	1.24
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	4	1.24
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	7	1.24
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD13	16	1.24
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	11	1.24
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	4	1.24
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	2	1.24
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	7	1.24
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	7	1.24
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	8	1.24
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	11	1.24
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	14	1.24
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	15	1.24
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG11	10	1.24
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG22	16	1.24
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	4	1.24
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	8	1.24
(1,869)	1:55:A:THR:HG22	1:68:A:SER:HB3	7	1.24
(1,866)	1:55:A:THR:HG22	1:56:A:CYS:HB2	12	1.24
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	14	1.24
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	14	1.24
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	18	1.24
(1,706)	1:44:A:ALA:HB1	1:64:A:TYR:HD1	14	1.24
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	17	1.24
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	9	1.24
(1,607)	1:36:A:THR:H	1:36:A:THR:HG21	3	1.24
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	17	1.24
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	19	1.24
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG22	9	1.24
(1,306)	1:18:A:THR:HG23	1:20:A:LYS:HA	15	1.24
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	16	1.24
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	18	1.24
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	9	1.24
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	17	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	3	1.24
(1,23)	1:78:A:CYS:HB2	1:70:A:PRO:HD3	6	1.24
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	17	1.23
(1,1745)	1:57:A:GLY:H	1:65:A:TYR:HD1	6	1.23
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	2	1.23
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	16	1.23
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	13	1.23
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	14	1.23
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	8	1.23
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	10	1.23
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	4	1.23
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	11	1.23
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	11	1.23
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	15	1.23
(1,1319)	1:79:A:GLN:HG3	1:80:A:LEU:HD23	1	1.23
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	12	1.23
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	13	1.23
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	14	1.23
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	2	1.23
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	4	1.23
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	5	1.23
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	16	1.23
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	17	1.23
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	18	1.23
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	15	1.23
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	2	1.23
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	3	1.23
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	1	1.23
(1,952)	1:59:A:VAL:HG12	1:58:A:TYR:HD1	5	1.23
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG11	14	1.23
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	10	1.23
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	17	1.23
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	4	1.23
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	17	1.23
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	4	1.23
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	5	1.23
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	1	1.23
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	1	1.23
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	3	1.23
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	10	1.23
(1,497)	1:67:A:CYS:HB2	1:50:A:CYS:HB3	8	1.23
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	8	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	19	1.23
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	14	1.23
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG21	15	1.23
(1,306)	1:18:A:THR:HG23	1:20:A:LYS:HA	12	1.23
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	2	1.23
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	18	1.23
(1,176)	1:7:A:PRO:HG2	1:21:A:LYS:HG3	16	1.23
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	1	1.23
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	14	1.23
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	20	1.23
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	20	1.22
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	1	1.22
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	1	1.22
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	4	1.22
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	10	1.22
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	7	1.22
(1,1399)	1:77:A:GLN:HB3	1:76:A:LYS:HA	5	1.22
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	9	1.22
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	3	1.22
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	11	1.22
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	14	1.22
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	19	1.22
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	1	1.22
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	13	1.22
(1,1182)	1:72:A:GLY:HA2	1:71:A:TYR:HD1	1	1.22
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	9	1.22
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	13	1.22
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	17	1.22
(1,1028)	1:59:A:VAL:HG12	1:64:A:TYR:HB3	6	1.22
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	18	1.22
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	11	1.22
(1,965)	1:59:A:VAL:HG21	1:64:A:TYR:H	18	1.22
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG23	2	1.22
(1,953)	1:59:A:VAL:HG13	1:60:A:TYR:HD1	1	1.22
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	19	1.22
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	4	1.22
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	8	1.22
(1,893)	1:57:A:GLY:HA3	1:58:A:TYR:HB3	14	1.22
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	19	1.22
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	20	1.22
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	19	1.22
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	20	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	3	1.22
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	19	1.22
(1,497)	1:67:A:CYS:HB2	1:50:A:CYS:HB3	4	1.22
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	3	1.22
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	5	1.22
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	1	1.22
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	17	1.22
(1,351)	1:20:A:LYS:HG2	1:21:A:LYS:H	7	1.22
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	5	1.22
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	15	1.22
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	4	1.22
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	3	1.22
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	20	1.22
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	12	1.22
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	9	1.22
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE2	6	1.22
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	11	1.22
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	10	1.21
(1,1645)	1:35:A:TYR:H	1:33:A:LYS:HG2	20	1.21
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	19	1.21
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	16	1.21
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	17	1.21
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	10	1.21
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	9	1.21
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	3	1.21
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	6	1.21
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	17	1.21
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	2	1.21
(1,1005)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	18	1.21
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	9	1.21
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG11	5	1.21
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG13	20	1.21
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	16	1.21
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	9	1.21
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	19	1.21
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	1	1.21
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	10	1.21
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	8	1.21
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	11	1.21
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	6	1.21
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	3	1.21
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	4	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	19	1.21
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	4	1.21
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	6	1.21
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	19	1.21
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	5	1.21
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	7	1.21
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HD2	4	1.21
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	20	1.21
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	3	1.2
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	4	1.2
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	15	1.2
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	12	1.2
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	14	1.2
(1,1445)	1:36:A:THR:HB	1:37:A:GLY:HA2	20	1.2
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	7	1.2
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	6	1.2
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	14	1.2
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	12	1.2
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	20	1.2
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD23	17	1.2
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD21	10	1.2
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD22	20	1.2
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	7	1.2
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	10	1.2
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	16	1.2
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	20	1.2
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	10	1.2
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	8	1.2
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	19	1.2
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	15	1.2
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	7	1.2
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	18	1.2
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	19	1.2
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	19	1.2
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	17	1.2
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG22	18	1.2
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	14	1.2
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	17	1.2
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG23	6	1.2
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG22	8	1.2
(1,960)	1:59:A:VAL:HG21	1:60:A:TYR:HB2	14	1.2
(1,943)	1:59:A:VAL:HG11	1:65:A:TYR:HB3	1	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,869)	1:55:A:THR:HG22	1:68:A:SER:HB3	1	1.2
(1,861)	1:55:A:THR:HB	1:68:A:SER:HA	12	1.2
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	10	1.2
(1,706)	1:44:A:ALA:HB1	1:64:A:TYR:HD1	18	1.2
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	2	1.2
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	4	1.2
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	11	1.2
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	7	1.2
(1,607)	1:36:A:THR:H	1:36:A:THR:HG21	17	1.2
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	4	1.2
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	19	1.2
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	12	1.2
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	3	1.2
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	11	1.2
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	7	1.2
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	10	1.2
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	12	1.2
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	13	1.2
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	10	1.2
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	15	1.2
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	19	1.2
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	16	1.2
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	19	1.2
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	16	1.2
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	3	1.2
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	15	1.2
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	6	1.19
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	9	1.19
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	12	1.19
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD23	17	1.19
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	15	1.19
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	5	1.19
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	7	1.19
(1,1379)	1:82:A:LYS:HE2	1:74:A:TYR:HE1	3	1.19
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	16	1.19
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD21	16	1.19
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	12	1.19
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	10	1.19
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	17	1.19
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	15	1.19
(1,1027)	1:59:A:VAL:HG12	1:64:A:TYR:HB2	6	1.19
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	13	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG22	1	1.19
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG23	3	1.19
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG21	4	1.19
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG21	7	1.19
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG21	18	1.19
(1,953)	1:59:A:VAL:HG12	1:60:A:TYR:HD1	15	1.19
(1,953)	1:59:A:VAL:HG11	1:60:A:TYR:HD1	18	1.19
(1,952)	1:59:A:VAL:HG11	1:58:A:TYR:HD1	16	1.19
(1,948)	1:59:A:VAL:HG13	1:64:A:TYR:HA	19	1.19
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG13	15	1.19
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG11	16	1.19
(1,943)	1:59:A:VAL:HG12	1:65:A:TYR:HB3	6	1.19
(1,940)	1:59:A:VAL:HG12	1:66:A:LYS:HG2	20	1.19
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	16	1.19
(1,866)	1:55:A:THR:HG22	1:56:A:CYS:HB2	15	1.19
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	10	1.19
(1,703)	1:44:A:ALA:HB2	1:58:A:TYR:HA	19	1.19
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	2	1.19
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	19	1.19
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	3	1.19
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	12	1.19
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	17	1.19
(1,599)	1:36:A:THR:HG23	1:64:A:TYR:HB3	5	1.19
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	9	1.19
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	8	1.19
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	5	1.19
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	7	1.19
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG21	10	1.19
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	3	1.19
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	14	1.19
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	17	1.19
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	19	1.19
(1,302)	1:18:A:THR:HG22	1:20:A:LYS:HD2	14	1.19
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	8	1.19
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	15	1.19
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	4	1.19
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	15	1.19
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	18	1.19
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE3	18	1.19
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	19	1.19
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	1	1.19
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	7	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	14	1.18
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	8	1.18
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	18	1.18
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	10	1.18
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	12	1.18
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	12	1.18
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	8	1.18
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	10	1.18
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	15	1.18
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	19	1.18
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	19	1.18
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	12	1.18
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD11	16	1.18
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	9	1.18
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	6	1.18
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	17	1.18
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	15	1.18
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	6	1.18
(1,1019)	1:64:A:TYR:HA	1:63:A:PRO:HB3	11	1.18
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG23	10	1.18
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG22	12	1.18
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG22	19	1.18
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG11	17	1.18
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	9	1.18
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	11	1.18
(1,869)	1:55:A:THR:HG23	1:68:A:SER:HB3	15	1.18
(1,866)	1:55:A:THR:HG23	1:56:A:CYS:HB2	16	1.18
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	6	1.18
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	4	1.18
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	12	1.18
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	11	1.18
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	9	1.18
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	6	1.18
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	2	1.18
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	10	1.18
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	9	1.18
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG13	3	1.18
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	1	1.18
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG22	7	1.18
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	13	1.18
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	11	1.18
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	2	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	15	1.18
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	15	1.18
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	9	1.18
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	5	1.18
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG22	6	1.18
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	1	1.18
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	2	1.18
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	14	1.18
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	17	1.18
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	2	1.18
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	2	1.18
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	13	1.17
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	1	1.17
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	14	1.17
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD13	3	1.17
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	17	1.17
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	10	1.17
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	9	1.17
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	17	1.17
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	2	1.17
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	16	1.17
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	5	1.17
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	17	1.17
(1,991)	1:64:A:TYR:H	1:62:A:TYR:HA	20	1.17
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	17	1.17
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG23	5	1.17
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG23	13	1.17
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	12	1.17
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	13	1.17
(1,869)	1:55:A:THR:HG21	1:68:A:SER:HB3	20	1.17
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	13	1.17
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	2	1.17
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	16	1.17
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	5	1.17
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	10	1.17
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	16	1.17
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	2	1.17
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	2	1.17
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG21	5	1.17
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	14	1.17
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	6	1.17
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	11	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	11	1.17
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	4	1.17
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	19	1.17
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	9	1.17
(1,306)	1:18:A:THR:HG21	1:20:A:LYS:HA	6	1.17
(1,306)	1:18:A:THR:HG21	1:20:A:LYS:HA	9	1.17
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	1	1.17
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	4	1.17
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	3	1.17
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	15	1.17
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	3	1.17
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	9	1.17
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	10	1.17
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	14	1.17
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	19	1.17
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	4	1.16
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	13	1.16
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	5	1.16
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	16	1.16
(1,1634)	1:34:A:GLY:H	1:33:A:LYS:HG2	20	1.16
(1,1523)	1:14:A:ARG:H	1:14:A:ARG:HG2	2	1.16
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	3	1.16
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	1	1.16
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	18	1.16
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	3	1.16
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	6	1.16
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	11	1.16
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	11	1.16
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	15	1.16
(1,1325)	1:66:A:LYS:HA	1:65:A:TYR:H	19	1.16
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	7	1.16
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	13	1.16
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	9	1.16
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	4	1.16
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	10	1.16
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	12	1.16
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG23	8	1.16
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG22	14	1.16
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	20	1.16
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG21	9	1.16
(1,962)	1:59:A:VAL:HG21	1:65:A:TYR:H	9	1.16
(1,952)	1:59:A:VAL:HG11	1:58:A:TYR:HD1	2	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:55:A:THR:HG21	1:56:A:CYS:HB2	8	1.16
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	18	1.16
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	3	1.16
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	9	1.16
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	14	1.16
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	6	1.16
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	2	1.16
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	15	1.16
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	14	1.16
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG22	7	1.16
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	13	1.16
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	19	1.16
(1,217)	1:9:A:SER:HA	1:10:A:PRO:HB2	5	1.16
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	15	1.16
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	12	1.16
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG21	12	1.16
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	2	1.16
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	4	1.16
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	2	1.16
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	10	1.16
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	18	1.15
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	9	1.15
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	9	1.15
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	1	1.15
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	14	1.15
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	14	1.15
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	14	1.15
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	6	1.15
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD13	20	1.15
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	10	1.15
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	5	1.15
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	6	1.15
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	11	1.15
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	10	1.15
(1,1185)	1:72:A:GLY:HA3	1:71:A:TYR:HD1	15	1.15
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	5	1.15
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	19	1.15
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	12	1.15
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	3	1.15
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	1	1.15
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	3	1.15
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	8	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	20	1.15
(1,866)	1:55:A:THR:HG23	1:56:A:CYS:HB2	2	1.15
(1,866)	1:55:A:THR:HG23	1:56:A:CYS:HB2	9	1.15
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	2	1.15
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	1	1.15
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	8	1.15
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	19	1.15
(1,706)	1:44:A:ALA:HB2	1:64:A:TYR:HD1	2	1.15
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	18	1.15
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	13	1.15
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG23	11	1.15
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG21	13	1.15
(1,453)	1:22:A:ARG:HG2	1:27:A:TYR:HA	6	1.15
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	18	1.15
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	3	1.15
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	5	1.15
(1,306)	1:18:A:THR:HG22	1:20:A:LYS:HA	18	1.15
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	20	1.15
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	11	1.15
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	15	1.15
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	19	1.15
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	16	1.15
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	7	1.15
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	13	1.15
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	12	1.15
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	1	1.14
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	10	1.14
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	17	1.14
(1,1508)	1:4:A:TYR:H	1:4:A:TYR:HD1	13	1.14
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	5	1.14
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	13	1.14
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	20	1.14
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	3	1.14
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	5	1.14
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD23	19	1.14
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD13	11	1.14
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	2	1.14
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	12	1.14
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	19	1.14
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	15	1.14
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	18	1.14
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	18	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	6	1.14
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG22	9	1.14
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	9	1.14
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	2	1.14
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	7	1.14
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	10	1.14
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	15	1.14
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG22	17	1.14
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	14	1.14
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	5	1.14
(1,866)	1:55:A:THR:HG23	1:56:A:CYS:HB2	11	1.14
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	5	1.14
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	20	1.14
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	7	1.14
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	16	1.14
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	19	1.14
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	10	1.14
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	19	1.14
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	8	1.14
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	14	1.14
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	4	1.14
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	1	1.14
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	7	1.14
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	13	1.14
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	18	1.14
(1,306)	1:18:A:THR:HG21	1:20:A:LYS:HA	4	1.14
(1,306)	1:18:A:THR:HG23	1:20:A:LYS:HA	20	1.14
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	3	1.14
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	4	1.14
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	2	1.14
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	15	1.14
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	6	1.14
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	17	1.13
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	20	1.13
(1,1645)	1:35:A:TYR:H	1:33:A:LYS:HG2	12	1.13
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	16	1.13
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	14	1.13
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	16	1.13
(1,1379)	1:82:A:LYS:HE2	1:74:A:TYR:HE1	14	1.13
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	12	1.13
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	10	1.13
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	14	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	2	1.13
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	19	1.13
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	19	1.13
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	9	1.13
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	13	1.13
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	15	1.13
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	4	1.13
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	2	1.13
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	18	1.13
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG21	10	1.13
(1,1005)	1:59:A:VAL:HG11	1:63:A:PRO:HD2	10	1.13
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	3	1.13
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	12	1.13
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	16	1.13
(1,953)	1:59:A:VAL:HG12	1:60:A:TYR:HD1	4	1.13
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	17	1.13
(1,869)	1:55:A:THR:HG21	1:68:A:SER:HB3	13	1.13
(1,866)	1:55:A:THR:HG21	1:56:A:CYS:HB2	18	1.13
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	11	1.13
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	7	1.13
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	19	1.13
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	2	1.13
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	9	1.13
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	14	1.13
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	4	1.13
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	12	1.13
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	15	1.13
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	11	1.13
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	16	1.13
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	7	1.13
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	14	1.13
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	10	1.13
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	15	1.13
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	9	1.13
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	7	1.13
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	5	1.13
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	8	1.13
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	13	1.13
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	17	1.13
(1,83)	1:2:A:VAL:HG23	1:4:A:TYR:HE1	10	1.13
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	15	1.13
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	20	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	1:44:A:ALA:HB3	1:58:A:TYR:HE1	10	1.12
(1,1436)	1:44:A:ALA:HB2	1:58:A:TYR:HE1	13	1.12
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	10	1.12
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	16	1.12
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	4	1.12
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	7	1.12
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	17	1.12
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	5	1.12
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	7	1.12
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	11	1.12
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG21	9	1.12
(1,965)	1:59:A:VAL:HG23	1:64:A:TYR:H	10	1.12
(1,960)	1:59:A:VAL:HG22	1:60:A:TYR:HB2	16	1.12
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	4	1.12
(1,866)	1:55:A:THR:HG23	1:56:A:CYS:HB2	13	1.12
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	2	1.12
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	14	1.12
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	19	1.12
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	14	1.12
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	14	1.12
(1,599)	1:36:A:THR:HG22	1:64:A:TYR:HB3	15	1.12
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	14	1.12
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	1	1.12
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	2	1.12
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	2	1.12
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	13	1.12
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	17	1.12
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	3	1.12
(1,307)	1:18:A:THR:HG21	1:30:A:TYR:HE1	9	1.12
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	18	1.12
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	1	1.12
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	10	1.12
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	20	1.12
(1,38)	1:82:A:LYS:H	1:74:A:TYR:HE1	15	1.12
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	1	1.12
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	18	1.11
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	15	1.11
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	13	1.11
(1,1698)	1:44:A:ALA:H	1:58:A:TYR:HE1	10	1.11
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	1	1.11
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	7	1.11
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	8	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	11	1.11
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	12	1.11
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	15	1.11
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	16	1.11
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	19	1.11
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	15	1.11
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	13	1.11
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	18	1.11
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	18	1.11
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	13	1.11
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	9	1.11
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	11	1.11
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	2	1.11
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	8	1.11
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	12	1.11
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	20	1.11
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	13	1.11
(1,1182)	1:72:A:GLY:HA2	1:71:A:TYR:HD1	8	1.11
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	7	1.11
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	8	1.11
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG23	16	1.11
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	2	1.11
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	4	1.11
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	6	1.11
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	1	1.11
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	5	1.11
(1,963)	1:59:A:VAL:H	1:59:A:VAL:HG23	20	1.11
(1,953)	1:59:A:VAL:HG12	1:60:A:TYR:HD1	19	1.11
(1,952)	1:59:A:VAL:HG11	1:58:A:TYR:HD1	20	1.11
(1,866)	1:55:A:THR:HG21	1:56:A:CYS:HB2	1	1.11
(1,866)	1:55:A:THR:HG22	1:56:A:CYS:HB2	3	1.11
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	8	1.11
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	13	1.11
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	13	1.11
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	4	1.11
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	18	1.11
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	5	1.11
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	8	1.11
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	13	1.11
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	12	1.11
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	13	1.11
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	5	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	16	1.11
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	12	1.11
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	17	1.11
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	5	1.11
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	9	1.11
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	7	1.11
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	2	1.11
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	16	1.11
(1,115)	1:6:A:ASN:H	1:5:A:PRO:HA	11	1.11
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	8	1.11
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	16	1.11
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	5	1.1
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	3	1.1
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	8	1.1
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	2	1.1
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	6	1.1
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	8	1.1
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	2	1.1
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	9	1.1
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	20	1.1
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	4	1.1
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	10	1.1
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	15	1.1
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	14	1.1
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	10	1.1
(1,1185)	1:72:A:GLY:HA3	1:71:A:TYR:HD1	18	1.1
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	16	1.1
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	18	1.1
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	2	1.1
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	6	1.1
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	19	1.1
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	16	1.1
(1,952)	1:59:A:VAL:HG11	1:58:A:TYR:HD1	1	1.1
(1,952)	1:59:A:VAL:HG12	1:58:A:TYR:HD1	18	1.1
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	18	1.1
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	7	1.1
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	5	1.1
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	14	1.1
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	17	1.1
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	11	1.1
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	13	1.1
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	18	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	1	1.1
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	16	1.1
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG23	12	1.1
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG23	16	1.1
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	7	1.1
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	17	1.1
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	12	1.1
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	12	1.1
(1,255)	1:14:A:ARG:HA	1:14:A:ARG:HD2	13	1.1
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	16	1.1
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	17	1.1
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	4	1.1
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	5	1.1
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	11	1.1
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	3	1.1
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	4	1.1
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	11	1.1
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	7	1.1
(1,12)	1:34:A:GLY:HA3	1:58:A:TYR:HB3	1	1.1
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	14	1.09
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	3	1.09
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	6	1.09
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	13	1.09
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	18	1.09
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	3	1.09
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	16	1.09
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	1	1.09
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	5	1.09
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	13	1.09
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD23	13	1.09
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	14	1.09
(1,1166)	1:71:A:TYR:HA	1:71:A:TYR:HD1	19	1.09
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	20	1.09
(1,1114)	1:70:A:PRO:HA	1:71:A:TYR:HB3	4	1.09
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	2	1.09
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	12	1.09
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	3	1.09
(1,1018)	1:64:A:TYR:HA	1:59:A:VAL:HG23	20	1.09
(1,1004)	1:63:A:PRO:HD3	1:59:A:VAL:HG13	9	1.09
(1,965)	1:59:A:VAL:HG21	1:64:A:TYR:H	4	1.09
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	15	1.09
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	16	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	7	1.09
(1,827)	1:51:A:LEU:HD13	1:51:A:LEU:H	2	1.09
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	18	1.09
(1,703)	1:44:A:ALA:HB3	1:58:A:TYR:HA	3	1.09
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	1	1.09
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	14	1.09
(1,630)	1:38:A:LYS:HD2	1:38:A:LYS:HA	19	1.09
(1,599)	1:36:A:THR:HG23	1:64:A:TYR:HB3	1	1.09
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	17	1.09
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	17	1.09
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	19	1.09
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	18	1.09
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	19	1.09
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG21	3	1.09
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	8	1.09
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	6	1.09
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	9	1.09
(1,397)	1:22:A:ARG:HG2	1:24:A:LEU:H	5	1.09
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	8	1.09
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	14	1.09
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	2	1.09
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	2	1.09
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	5	1.09
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	6	1.09
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	18	1.09
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	15	1.09
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	16	1.09
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	18	1.09
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	11	1.09
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	19	1.09
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	1	1.09
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	19	1.09
(1,9)	1:31:A:CYS:HB2	1:32:A:ARG:HG2	8	1.09
(1,3)	1:83:A:TYR:HB2	1:82:A:LYS:HB3	7	1.09
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	13	1.08
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	7	1.08
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	17	1.08
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	10	1.08
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	4	1.08
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	17	1.08
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	1	1.08
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	19	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	10	1.08
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	2	1.08
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD22	15	1.08
(1,1300)	1:79:A:GLN:HG3	1:80:A:LEU:HB2	1	1.08
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	20	1.08
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD22	5	1.08
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	9	1.08
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	12	1.08
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	18	1.08
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	20	1.08
(1,940)	1:59:A:VAL:HG12	1:66:A:LYS:HG2	2	1.08
(1,940)	1:59:A:VAL:HG12	1:66:A:LYS:HG2	9	1.08
(1,866)	1:55:A:THR:HG23	1:56:A:CYS:HB2	20	1.08
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	16	1.08
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	2	1.08
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	7	1.08
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	8	1.08
(1,706)	1:44:A:ALA:HB3	1:64:A:TYR:HD1	4	1.08
(1,706)	1:44:A:ALA:HB2	1:64:A:TYR:HD1	17	1.08
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	7	1.08
(1,610)	1:61:A:GLY:HA2	1:62:A:TYR:HB2	5	1.08
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG22	6	1.08
(1,599)	1:36:A:THR:HG22	1:64:A:TYR:HB3	17	1.08
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	1	1.08
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	3	1.08
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	6	1.08
(1,497)	1:67:A:CYS:HB2	1:50:A:CYS:HB3	10	1.08
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	15	1.08
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	2	1.08
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	8	1.08
(1,442)	1:74:A:TYR:HA	1:80:A:LEU:HB2	9	1.08
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	1	1.08
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	12	1.08
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	15	1.08
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	10	1.08
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	3	1.08
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	10	1.08
(1,344)	1:18:A:THR:HG23	1:20:A:LYS:HE2	14	1.08
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	8	1.08
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	20	1.08
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	8	1.08
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	18	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:6:A:ASN:H	1:5:A:PRO:HA	18	1.08
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	12	1.08
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	19	1.08
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	14	1.08
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	6	1.08
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	15	1.08
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE3	19	1.08
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	16	1.07
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD23	18	1.07
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD22	19	1.07
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	7	1.07
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	16	1.07
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	6	1.07
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	15	1.07
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	9	1.07
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	20	1.07
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	3	1.07
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	9	1.07
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG12	8	1.07
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	15	1.07
(1,866)	1:55:A:THR:HG22	1:56:A:CYS:HB2	17	1.07
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	10	1.07
(1,827)	1:51:A:LEU:HD12	1:51:A:LEU:H	7	1.07
(1,706)	1:44:A:ALA:HB3	1:64:A:TYR:HD1	6	1.07
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	5	1.07
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	12	1.07
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	6	1.07
(1,647)	1:39:A:ASN:HB2	1:41:A:GLN:HB3	2	1.07
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	5	1.07
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	15	1.07
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	7	1.07
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	12	1.07
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	6	1.07
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	16	1.07
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	9	1.07
(1,401)	1:23:A:GLY:HA3	1:24:A:LEU:HD23	7	1.07
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	7	1.07
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	2	1.07
(1,326)	1:20:A:LYS:HB3	1:22:A:ARG:HD2	17	1.07
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	1	1.07
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	3	1.07
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	4	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	10	1.07
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	12	1.07
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	16	1.07
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	8	1.07
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	8	1.07
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	5	1.07
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	15	1.07
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	2	1.07
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	12	1.07
(1,115)	1:6:A:ASN:H	1:5:A:PRO:HA	14	1.07
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	19	1.07
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	11	1.07
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	9	1.06
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	2	1.06
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	9	1.06
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	11	1.06
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	1	1.06
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	4	1.06
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	7	1.06
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	14	1.06
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	10	1.06
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	20	1.06
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	12	1.06
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	16	1.06
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	9	1.06
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	4	1.06
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG12	12	1.06
(1,952)	1:59:A:VAL:HG13	1:58:A:TYR:HD1	4	1.06
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	5	1.06
(1,869)	1:55:A:THR:HG21	1:68:A:SER:HB3	2	1.06
(1,865)	1:55:A:THR:HG23	1:56:A:CYS:HB3	16	1.06
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	5	1.06
(1,838)	1:53:A:GLY:HA2	1:70:A:PRO:HG3	12	1.06
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	11	1.06
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	16	1.06
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	4	1.06
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	2	1.06
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	3	1.06
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG22	18	1.06
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG21	2	1.06
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	6	1.06
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	17	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	18	1.06
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	12	1.06
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	1	1.06
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	9	1.06
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	15	1.06
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	19	1.06
(1,166)	1:7:A:PRO:HD3	1:21:A:LYS:HG3	6	1.06
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	4	1.06
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	9	1.06
(1,23)	1:78:A:CYS:HB2	1:70:A:PRO:HD3	9	1.06
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	20	1.06
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	17	1.05
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	14	1.05
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	2	1.05
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	10	1.05
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	18	1.05
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	15	1.05
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	10	1.05
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	5	1.05
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD12	13	1.05
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	9	1.05
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	20	1.05
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	1	1.05
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	8	1.05
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	11	1.05
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	14	1.05
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	14	1.05
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG23	17	1.05
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	1	1.05
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG13	7	1.05
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	11	1.05
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	7	1.05
(1,866)	1:55:A:THR:HG23	1:56:A:CYS:HB2	10	1.05
(1,866)	1:55:A:THR:HG22	1:56:A:CYS:HB2	14	1.05
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	8	1.05
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	2	1.05
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	9	1.05
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	11	1.05
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	17	1.05
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB3	12	1.05
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	14	1.05
(1,599)	1:36:A:THR:HG23	1:64:A:TYR:HB3	14	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	17	1.05
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	14	1.05
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	17	1.05
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG23	12	1.05
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG23	16	1.05
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	12	1.05
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	10	1.05
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	9	1.05
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	11	1.05
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	13	1.05
(1,285)	1:18:A:THR:HA	1:19:A:CYS:HA	14	1.05
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	1	1.05
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	1	1.05
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	2	1.05
(1,89)	1:3:A:TYR:HA	1:3:A:TYR:HD1	12	1.05
(1,26)	1:79:A:GLN:HB2	1:50:A:CYS:HA	15	1.05
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	8	1.05
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	14	1.04
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	18	1.04
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	20	1.04
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	1	1.04
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	2	1.04
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	17	1.04
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	17	1.04
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	17	1.04
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	17	1.04
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	9	1.04
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	15	1.04
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	3	1.04
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD12	11	1.04
(1,1300)	1:79:A:GLN:HG3	1:80:A:LEU:HB2	7	1.04
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	3	1.04
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD22	11	1.04
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	15	1.04
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	2	1.04
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	1	1.04
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	9	1.04
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	10	1.04
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	11	1.04
(1,1166)	1:71:A:TYR:HA	1:71:A:TYR:HD1	3	1.04
(1,1135)	1:72:A:GLY:H	1:70:A:PRO:HB3	14	1.04
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	11	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	1	1.04
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	13	1.04
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	16	1.04
(1,988)	1:62:A:TYR:HA	1:62:A:TYR:HD1	6	1.04
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG11	2	1.04
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	6	1.04
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	16	1.04
(1,869)	1:55:A:THR:HG21	1:68:A:SER:HB3	9	1.04
(1,869)	1:55:A:THR:HG21	1:68:A:SER:HB3	11	1.04
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	9	1.04
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	17	1.04
(1,703)	1:44:A:ALA:HB3	1:58:A:TYR:HA	9	1.04
(1,697)	1:44:A:ALA:HB1	1:34:A:GLY:HA2	17	1.04
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	8	1.04
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG22	7	1.04
(1,599)	1:36:A:THR:HG21	1:64:A:TYR:HB3	11	1.04
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	13	1.04
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	3	1.04
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	10	1.04
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	20	1.04
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG21	10	1.04
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	17	1.04
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	3	1.04
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	9	1.04
(1,306)	1:18:A:THR:HG22	1:20:A:LYS:HA	11	1.04
(1,295)	1:18:A:THR:HB	1:19:A:CYS:HA	17	1.04
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	11	1.04
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	15	1.04
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	16	1.04
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG21	15	1.04
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	3	1.04
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	5	1.04
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	7	1.04
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE3	8	1.04
(1,1882)	1:2:A:VAL:H	1:2:A:VAL:HG11	10	1.03
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	14	1.03
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	20	1.03
(1,1493)	1:2:A:VAL:HG11	1:4:A:TYR:HD1	13	1.03
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	6	1.03
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	13	1.03
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	17	1.03
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	18	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:47:A:PRO:HB2	1:46:A:PHE:HB3	4	1.03
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	12	1.03
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	20	1.03
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	9	1.03
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	18	1.03
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD23	5	1.03
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD22	5	1.03
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	8	1.03
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD13	8	1.03
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD12	16	1.03
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD22	19	1.03
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	16	1.03
(1,1208)	1:75:A:GLY:HA2	1:76:A:LYS:HB2	15	1.03
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	20	1.03
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	16	1.03
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	5	1.03
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	12	1.03
(1,866)	1:55:A:THR:HG23	1:56:A:CYS:HB2	5	1.03
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	2	1.03
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	15	1.03
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	2	1.03
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	5	1.03
(1,703)	1:44:A:ALA:HB2	1:58:A:TYR:HA	15	1.03
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB1	3	1.03
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	12	1.03
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	10	1.03
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG23	13	1.03
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	8	1.03
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	3	1.03
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	20	1.03
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	18	1.03
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	15	1.03
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG21	6	1.03
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	19	1.03
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	12	1.03
(1,305)	1:18:A:THR:HG22	1:17:A:GLY:HA2	13	1.03
(1,279)	1:17:A:GLY:HA3	1:18:A:THR:HB	12	1.03
(1,256)	1:14:A:ARG:HD2	1:14:A:ARG:H	13	1.03
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	18	1.03
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	4	1.03
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	2	1.03
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	7	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	15	1.03
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	12	1.03
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	7	1.03
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	11	1.02
(1,1789)	1:67:A:CYS:H	1:65:A:TYR:HD1	18	1.02
(1,1700)	1:45:A:CYS:H	1:46:A:PHE:HB2	18	1.02
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD23	1	1.02
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	2	1.02
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	10	1.02
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	1	1.02
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	18	1.02
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	16	1.02
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	10	1.02
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	19	1.02
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	8	1.02
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	12	1.02
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD12	4	1.02
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	7	1.02
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	13	1.02
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	5	1.02
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	6	1.02
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	16	1.02
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	18	1.02
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	11	1.02
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	7	1.02
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	7	1.02
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	13	1.02
(1,965)	1:59:A:VAL:HG22	1:64:A:TYR:H	19	1.02
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	1	1.02
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	18	1.02
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	15	1.02
(1,641)	1:39:A:ASN:HA	1:29:A:CYS:HB3	11	1.02
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	8	1.02
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	15	1.02
(1,497)	1:67:A:CYS:HB2	1:50:A:CYS:HB3	15	1.02
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	9	1.02
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	12	1.02
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	5	1.02
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	18	1.02
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	19	1.02
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	4	1.02
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	17	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	9	1.02
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	13	1.02
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	8	1.02
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	20	1.02
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	11	1.02
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	1	1.02
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	3	1.02
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	12	1.01
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	11	1.01
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	13	1.01
(1,1500)	1:51:A:LEU:HD23	1:50:A:CYS:H	3	1.01
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	3	1.01
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	8	1.01
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	20	1.01
(1,1467)	1:22:A:ARG:HD2	1:22:A:ARG:H	5	1.01
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	9	1.01
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	10	1.01
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	1	1.01
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	7	1.01
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	19	1.01
(1,1337)	1:81:A:LYS:HB2	1:83:A:TYR:HE1	13	1.01
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	3	1.01
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	16	1.01
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD13	4	1.01
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	13	1.01
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	2	1.01
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	6	1.01
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	2	1.01
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	19	1.01
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	20	1.01
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG13	3	1.01
(1,866)	1:55:A:THR:HG21	1:56:A:CYS:HB2	7	1.01
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	1	1.01
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	18	1.01
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	3	1.01
(1,706)	1:44:A:ALA:HB3	1:64:A:TYR:HD1	13	1.01
(1,698)	1:44:A:ALA:HB2	1:65:A:TYR:HB2	10	1.01
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	17	1.01
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	13	1.01
(1,635)	1:38:A:LYS:HG3	1:38:A:LYS:HE2	19	1.01
(1,592)	1:36:A:THR:HB	1:44:A:ALA:HB2	16	1.01
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	8	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	15	1.01
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG23	8	1.01
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	20	1.01
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG22	4	1.01
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	18	1.01
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	15	1.01
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	3	1.01
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	10	1.01
(1,263)	1:15:A:ASN:HB2	1:16:A:GLY:HA2	7	1.01
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	9	1.01
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	12	1.01
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	17	1.01
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	18	1.01
(1,239)	1:13:A:CYS:HA	1:14:A:ARG:HG2	13	1.01
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	5	1.01
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	14	1.01
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	4	1.01
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	4	1.01
(1,83)	1:2:A:VAL:HG22	1:4:A:TYR:HE1	11	1.01
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	2	1.01
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	15	1.0
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	16	1.0
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	10	1.0
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	5	1.0
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	5	1.0
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	5	1.0
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	10	1.0
(1,1373)	1:72:A:GLY:HA2	1:82:A:LYS:HD2	16	1.0
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	6	1.0
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD21	18	1.0
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	9	1.0
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD12	15	1.0
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	1	1.0
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	15	1.0
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	15	1.0
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	1	1.0
(1,952)	1:59:A:VAL:HG13	1:58:A:TYR:HD1	19	1.0
(1,865)	1:55:A:THR:HG23	1:56:A:CYS:HB3	11	1.0
(1,865)	1:55:A:THR:HG22	1:56:A:CYS:HB3	12	1.0
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	16	1.0
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	19	1.0
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	12	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	1:44:A:ALA:HB1	1:64:A:TYR:HD1	1	1.0
(1,703)	1:44:A:ALA:HB3	1:58:A:TYR:HA	18	1.0
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB3	10	1.0
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB1	17	1.0
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB1	18	1.0
(1,674)	1:42:A:TYR:HA	1:42:A:TYR:HD1	18	1.0
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	3	1.0
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	3	1.0
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	14	1.0
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	16	1.0
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	12	1.0
(1,580)	1:35:A:TYR:HA	1:35:A:TYR:HD1	6	1.0
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	1	1.0
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	5	1.0
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	9	1.0
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	10	1.0
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	1	1.0
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	14	1.0
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	8	1.0
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	11	1.0
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	2	1.0
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	16	1.0
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	13	1.0
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	1	1.0
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	3	1.0
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	17	1.0
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	17	1.0
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	1	0.99
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	4	0.99
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	20	0.99
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	4	0.99
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	17	0.99
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	3	0.99
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	10	0.99
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	20	0.99
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	1	0.99
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	6	0.99
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	7	0.99
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	10	0.99
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	12	0.99
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	19	0.99
(1,1422)	1:56:A:CYS:HB3	1:45:A:CYS:HB3	10	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	20	0.99
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	19	0.99
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD21	20	0.99
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD13	13	0.99
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	8	0.99
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	8	0.99
(1,1185)	1:72:A:GLY:HA3	1:71:A:TYR:HD1	2	0.99
(1,1182)	1:72:A:GLY:HA2	1:71:A:TYR:HD1	17	0.99
(1,1127)	1:70:A:PRO:HB3	1:71:A:TYR:HA	14	0.99
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	12	0.99
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	13	0.99
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	10	0.99
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	15	0.99
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	4	0.99
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	18	0.99
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG23	11	0.99
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG23	12	0.99
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	20	0.99
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	8	0.99
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	10	0.99
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	3	0.99
(1,869)	1:55:A:THR:HG21	1:68:A:SER:HB3	16	0.99
(1,827)	1:51:A:LEU:HD12	1:51:A:LEU:H	17	0.99
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	20	0.99
(1,706)	1:44:A:ALA:HB1	1:64:A:TYR:HD1	8	0.99
(1,706)	1:44:A:ALA:HB1	1:64:A:TYR:HD1	9	0.99
(1,706)	1:44:A:ALA:HB3	1:64:A:TYR:HD1	11	0.99
(1,703)	1:44:A:ALA:HB3	1:58:A:TYR:HA	1	0.99
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB3	9	0.99
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB3	19	0.99
(1,697)	1:44:A:ALA:HB3	1:34:A:GLY:HA2	18	0.99
(1,695)	1:44:A:ALA:HB3	1:45:A:CYS:HB3	20	0.99
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	8	0.99
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	11	0.99
(1,646)	1:39:A:ASN:HB3	1:41:A:GLN:HA	14	0.99
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	9	0.99
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	1	0.99
(1,559)	1:33:A:LYS:HG2	1:34:A:GLY:HA3	12	0.99
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	15	0.99
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	16	0.99
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	9	0.99
(1,472)	1:81:A:LYS:HA	1:83:A:TYR:HE1	18	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	18	0.99
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	19	0.99
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	17	0.99
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	16	0.99
(1,305)	1:18:A:THR:HG23	1:17:A:GLY:HA2	16	0.99
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	14	0.99
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	5	0.99
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	17	0.99
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	17	0.99
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	16	0.99
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	6	0.99
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	11	0.99
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	14	0.99
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	16	0.99
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	4	0.99
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	17	0.99
(1,12)	1:34:A:GLY:HA3	1:33:A:LYS:HE2	10	0.99
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	12	0.98
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	11	0.98
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	5	0.98
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	12	0.98
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	7	0.98
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	2	0.98
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	3	0.98
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	9	0.98
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	13	0.98
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	14	0.98
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	2	0.98
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	7	0.98
(1,1369)	1:82:A:LYS:HB3	1:83:A:TYR:HD1	15	0.98
(1,1337)	1:81:A:LYS:HB2	1:83:A:TYR:HE1	20	0.98
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	4	0.98
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	1	0.98
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	3	0.98
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	8	0.98
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG23	19	0.98
(1,1005)	1:59:A:VAL:HG13	1:63:A:PRO:HD2	9	0.98
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	12	0.98
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	8	0.98
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	15	0.98
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	19	0.98
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	15	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:55:A:THR:HG21	1:56:A:CYS:HB2	4	0.98
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	9	0.98
(1,600)	1:36:A:THR:HG22	1:64:A:TYR:HB2	16	0.98
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	4	0.98
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	19	0.98
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	10	0.98
(1,498)	1:29:A:CYS:HB3	1:28:A:LYS:HA	3	0.98
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	7	0.98
(1,305)	1:18:A:THR:HG21	1:17:A:GLY:HA2	1	0.98
(1,305)	1:18:A:THR:HG21	1:17:A:GLY:HA2	4	0.98
(1,305)	1:18:A:THR:HG21	1:17:A:GLY:HA2	6	0.98
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	11	0.98
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	6	0.98
(1,249)	1:13:A:CYS:HB2	1:11:A:TYR:HD1	11	0.98
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	9	0.98
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	19	0.98
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG21	17	0.98
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	10	0.98
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	13	0.98
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	18	0.98
(1,23)	1:78:A:CYS:HB2	1:70:A:PRO:HD3	11	0.98
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	10	0.98
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	14	0.97
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	15	0.97
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	6	0.97
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	19	0.97
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	9	0.97
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	5	0.97
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	7	0.97
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	11	0.97
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	14	0.97
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	4	0.97
(1,1468)	1:22:A:ARG:HB3	1:21:A:LYS:HA	15	0.97
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	5	0.97
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	11	0.97
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	2	0.97
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	15	0.97
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	16	0.97
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD11	20	0.97
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD13	6	0.97
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD11	13	0.97
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	10	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	2	0.97
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	3	0.97
(1,1171)	1:71:A:TYR:HB3	1:71:A:TYR:HE1	19	0.97
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	12	0.97
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	16	0.97
(1,1050)	1:65:A:TYR:HB3	1:58:A:TYR:HA	9	0.97
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	18	0.97
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	5	0.97
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG13	20	0.97
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	15	0.97
(1,873)	1:55:A:THR:H	1:55:A:THR:HG21	4	0.97
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	18	0.97
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	1	0.97
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	7	0.97
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	7	0.97
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	18	0.97
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	14	0.97
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG21	15	0.97
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	4	0.97
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	20	0.97
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	2	0.97
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	15	0.97
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	1	0.97
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	12	0.97
(1,95)	1:3:A:TYR:HB2	1:3:A:TYR:HD1	8	0.97
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	16	0.97
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	20	0.97
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	2	0.97
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	16	0.97
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	18	0.97
(1,9)	1:31:A:CYS:HB2	1:32:A:ARG:HG2	18	0.97
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	6	0.96
(1,1500)	1:51:A:LEU:HD23	1:50:A:CYS:H	12	0.96
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	16	0.96
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	18	0.96
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	14	0.96
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	6	0.96
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	10	0.96
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	11	0.96
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	3	0.96
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	15	0.96
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	9	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD21	3	0.96
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD11	2	0.96
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	8	0.96
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	15	0.96
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	5	0.96
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	6	0.96
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	10	0.96
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	10	0.96
(1,948)	1:59:A:VAL:HG11	1:64:A:TYR:HA	1	0.96
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	14	0.96
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	5	0.96
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	12	0.96
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	19	0.96
(1,873)	1:55:A:THR:H	1:55:A:THR:HG23	13	0.96
(1,865)	1:55:A:THR:HG21	1:56:A:CYS:HB3	19	0.96
(1,848)	1:54:A:GLY:HA2	1:69:A:CYS:HB2	13	0.96
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	8	0.96
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	18	0.96
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	20	0.96
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	18	0.96
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	17	0.96
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	4	0.96
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	18	0.96
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG22	4	0.96
(1,471)	1:66:A:LYS:HA	1:67:A:CYS:HB3	5	0.96
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	14	0.96
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	16	0.96
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	19	0.96
(1,305)	1:18:A:THR:HG21	1:17:A:GLY:HA2	8	0.96
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	14	0.96
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	8	0.96
(1,235)	1:11:A:TYR:HA	1:11:A:TYR:HD1	7	0.96
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	3	0.96
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	10	0.96
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	13	0.96
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	16	0.96
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	7	0.95
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	8	0.95
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD22	5	0.95
(1,1500)	1:51:A:LEU:HD22	1:50:A:CYS:H	19	0.95
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	18	0.95
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	5	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	1:44:A:ALA:HB2	1:58:A:TYR:HE1	6	0.95
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	7	0.95
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	8	0.95
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	4	0.95
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	19	0.95
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	11	0.95
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	18	0.95
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD23	15	0.95
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD21	14	0.95
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD23	18	0.95
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	7	0.95
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	3	0.95
(1,1050)	1:65:A:TYR:HB3	1:58:A:TYR:HA	12	0.95
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	17	0.95
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG12	7	0.95
(1,952)	1:59:A:VAL:HG12	1:58:A:TYR:HD1	6	0.95
(1,873)	1:55:A:THR:H	1:55:A:THR:HG23	10	0.95
(1,865)	1:55:A:THR:HG22	1:56:A:CYS:HB3	14	0.95
(1,865)	1:55:A:THR:HG22	1:56:A:CYS:HB3	15	0.95
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	11	0.95
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	20	0.95
(1,822)	1:51:A:LEU:HD23	1:56:A:CYS:HB3	18	0.95
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD22	6	0.95
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD21	14	0.95
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	2	0.95
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	6	0.95
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB1	20	0.95
(1,698)	1:44:A:ALA:HB3	1:65:A:TYR:HB2	17	0.95
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	3	0.95
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	10	0.95
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	17	0.95
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	3	0.95
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	13	0.95
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	14	0.95
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	20	0.95
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	12	0.95
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	17	0.95
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG23	19	0.95
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	19	0.95
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	7	0.95
(1,305)	1:18:A:THR:HG21	1:17:A:GLY:HA2	3	0.95
(1,305)	1:18:A:THR:HG23	1:17:A:GLY:HA2	9	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:18:A:THR:HG21	1:17:A:GLY:HA2	11	0.95
(1,235)	1:11:A:TYR:HA	1:11:A:TYR:HD1	13	0.95
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	10	0.95
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	5	0.95
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	9	0.95
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	17	0.95
(1,24)	1:78:A:CYS:HB3	1:70:A:PRO:HD3	15	0.95
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	6	0.95
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	3	0.95
(1,1860)	1:83:A:TYR:H	1:74:A:TYR:HD1	2	0.94
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	4	0.94
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	11	0.94
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	12	0.94
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	11	0.94
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	5	0.94
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	19	0.94
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	20	0.94
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	1	0.94
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	8	0.94
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	19	0.94
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	6	0.94
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	8	0.94
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	11	0.94
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD21	13	0.94
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	12	0.94
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	11	0.94
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	10	0.94
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	14	0.94
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	2	0.94
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	13	0.94
(1,1185)	1:72:A:GLY:HA3	1:71:A:TYR:HD1	4	0.94
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	18	0.94
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	7	0.94
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	11	0.94
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	16	0.94
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	4	0.94
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	14	0.94
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG12	10	0.94
(1,873)	1:55:A:THR:H	1:55:A:THR:HG21	6	0.94
(1,873)	1:55:A:THR:H	1:55:A:THR:HG23	9	0.94
(1,865)	1:55:A:THR:HG23	1:56:A:CYS:HB3	2	0.94
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD22	1	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD22	4	0.94
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD22	5	0.94
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD23	7	0.94
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD21	8	0.94
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD21	9	0.94
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD23	11	0.94
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD22	17	0.94
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	11	0.94
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	5	0.94
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	11	0.94
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	5	0.94
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	7	0.94
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	8	0.94
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	14	0.94
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	15	0.94
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	19	0.94
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	4	0.94
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	7	0.94
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	3	0.94
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	11	0.94
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	18	0.94
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG23	17	0.94
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	1	0.94
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	9	0.94
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	11	0.94
(1,305)	1:18:A:THR:HG21	1:17:A:GLY:HA2	14	0.94
(1,305)	1:18:A:THR:HG22	1:17:A:GLY:HA2	17	0.94
(1,305)	1:18:A:THR:HG21	1:17:A:GLY:HA2	18	0.94
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	9	0.94
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	4	0.94
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	10	0.94
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	5	0.94
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	11	0.94
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	20	0.94
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG21	14	0.94
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	6	0.94
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	16	0.94
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	12	0.94
(1,4)	1:7:A:PRO:HA	1:27:A:TYR:HB2	16	0.94
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	2	0.93
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	10	0.93
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	5	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	10	0.93
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	3	0.93
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	5	0.93
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	8	0.93
(1,1437)	1:44:A:ALA:HB2	1:36:A:THR:HG22	16	0.93
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	15	0.93
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	2	0.93
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	13	0.93
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	7	0.93
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	5	0.93
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	10	0.93
(1,1207)	1:75:A:GLY:HA2	1:76:A:LYS:HG3	7	0.93
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	12	0.93
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	14	0.93
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	1	0.93
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	4	0.93
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	3	0.93
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	15	0.93
(1,1023)	1:64:A:TYR:HA	1:64:A:TYR:HD1	19	0.93
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG13	12	0.93
(1,873)	1:55:A:THR:H	1:55:A:THR:HG21	1	0.93
(1,873)	1:55:A:THR:H	1:55:A:THR:HG23	2	0.93
(1,873)	1:55:A:THR:H	1:55:A:THR:HG21	19	0.93
(1,865)	1:55:A:THR:HG21	1:56:A:CYS:HB3	8	0.93
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	4	0.93
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	5	0.93
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD23	10	0.93
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD21	16	0.93
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD23	19	0.93
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	18	0.93
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	1	0.93
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	15	0.93
(1,698)	1:44:A:ALA:HB1	1:65:A:TYR:HB2	19	0.93
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	20	0.93
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	11	0.93
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	14	0.93
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	4	0.93
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	9	0.93
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	11	0.93
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	17	0.93
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG23	1	0.93
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	13	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	6	0.93
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	10	0.93
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	15	0.93
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	19	0.93
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	16	0.93
(1,400)	1:23:A:GLY:HA2	1:24:A:LEU:HB2	20	0.93
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	11	0.93
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	17	0.93
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	10	0.93
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	3	0.93
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	20	0.93
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	2	0.93
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	12	0.93
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	5	0.93
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	6	0.93
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	8	0.93
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	4	0.93
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	19	0.93
(1,12)	1:34:A:GLY:HA3	1:58:A:TYR:HB3	8	0.93
(1,12)	1:34:A:GLY:HA3	1:58:A:TYR:HB3	17	0.93
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	1	0.93
(1,1789)	1:67:A:CYS:H	1:65:A:TYR:HD1	12	0.92
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	13	0.92
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	1	0.92
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	16	0.92
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	8	0.92
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	5	0.92
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	13	0.92
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	17	0.92
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	7	0.92
(1,1373)	1:72:A:GLY:HA2	1:82:A:LYS:HD2	5	0.92
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	17	0.92
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	12	0.92
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	6	0.92
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	9	0.92
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	5	0.92
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	1	0.92
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	17	0.92
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	2	0.92
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	1	0.92
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	14	0.92
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	19	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	7	0.92
(1,873)	1:55:A:THR:H	1:55:A:THR:HG22	3	0.92
(1,873)	1:55:A:THR:H	1:55:A:THR:HG22	15	0.92
(1,873)	1:55:A:THR:H	1:55:A:THR:HG21	18	0.92
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	9	0.92
(1,847)	1:54:A:GLY:HA3	1:69:A:CYS:HB2	20	0.92
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD21	12	0.92
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD23	13	0.92
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD21	15	0.92
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD22	18	0.92
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD21	20	0.92
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	3	0.92
(1,690)	1:44:A:ALA:HA	1:58:A:TYR:HD1	17	0.92
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	19	0.92
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	1	0.92
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	9	0.92
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	15	0.92
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	16	0.92
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	11	0.92
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	15	0.92
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	5	0.92
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	10	0.92
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	14	0.92
(1,600)	1:36:A:THR:HG22	1:64:A:TYR:HB2	3	0.92
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	17	0.92
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	8	0.92
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	14	0.92
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	12	0.92
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	1	0.92
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	4	0.92
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	9	0.92
(1,305)	1:18:A:THR:HG23	1:17:A:GLY:HA2	19	0.92
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	20	0.92
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	11	0.92
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	7	0.92
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	20	0.92
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	14	0.92
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	12	0.92
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	13	0.92
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	18	0.92
(1,45)	1:11:A:TYR:HE1	1:19:A:CYS:HA	20	0.92
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	20	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE2	12	0.92
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	6	0.91
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	12	0.91
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	19	0.91
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	19	0.91
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	6	0.91
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	12	0.91
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	15	0.91
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	13	0.91
(1,1402)	1:80:A:LEU:HD22	1:75:A:GLY:HA3	19	0.91
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	17	0.91
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	2	0.91
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	5	0.91
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	10	0.91
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	3	0.91
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD11	3	0.91
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	8	0.91
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD23	20	0.91
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	20	0.91
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD11	16	0.91
(1,1182)	1:72:A:GLY:HA2	1:71:A:TYR:HD1	16	0.91
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	3	0.91
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	5	0.91
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	7	0.91
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	9	0.91
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	10	0.91
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	13	0.91
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	14	0.91
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	15	0.91
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	16	0.91
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	18	0.91
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	19	0.91
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	17	0.91
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	20	0.91
(1,1046)	1:59:A:VAL:H	1:65:A:TYR:HA	6	0.91
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	19	0.91
(1,1005)	1:59:A:VAL:HG13	1:63:A:PRO:HD2	20	0.91
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	6	0.91
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	6	0.91
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG13	2	0.91
(1,953)	1:59:A:VAL:HG13	1:60:A:TYR:HD1	16	0.91
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	14	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,873)	1:55:A:THR:H	1:55:A:THR:HG22	14	0.91
(1,873)	1:55:A:THR:H	1:55:A:THR:HG23	16	0.91
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	11	0.91
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	15	0.91
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	15	0.91
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	13	0.91
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD23	2	0.91
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	7	0.91
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	9	0.91
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	17	0.91
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB1	1	0.91
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB2	7	0.91
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB3	13	0.91
(1,697)	1:44:A:ALA:HB2	1:34:A:GLY:HA2	15	0.91
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	3	0.91
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	15	0.91
(1,657)	1:40:A:CYS:HB2	1:31:A:CYS:HB3	20	0.91
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	1	0.91
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	2	0.91
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	12	0.91
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	6	0.91
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	1	0.91
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG13	4	0.91
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	15	0.91
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	18	0.91
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	20	0.91
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	1	0.91
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	16	0.91
(1,305)	1:18:A:THR:HG21	1:17:A:GLY:HA2	2	0.91
(1,305)	1:18:A:THR:HG23	1:17:A:GLY:HA2	5	0.91
(1,305)	1:18:A:THR:HG22	1:17:A:GLY:HA2	15	0.91
(1,297)	1:18:A:THR:HB	1:30:A:TYR:HE1	11	0.91
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	19	0.91
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	7	0.91
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	9	0.91
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	5	0.91
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	14	0.91
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	16	0.91
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	14	0.91
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	19	0.91
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	14	0.9
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	15	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	9	0.9
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	3	0.9
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	13	0.9
(1,1439)	1:42:A:TYR:HB3	1:42:A:TYR:HD1	19	0.9
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	17	0.9
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	18	0.9
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	20	0.9
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD21	8	0.9
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	9	0.9
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD13	2	0.9
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	6	0.9
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	1	0.9
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	2	0.9
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	6	0.9
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	8	0.9
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	20	0.9
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	13	0.9
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	15	0.9
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	10	0.9
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	8	0.9
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	3	0.9
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	12	0.9
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	5	0.9
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	7	0.9
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	8	0.9
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	13	0.9
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	18	0.9
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG12	15	0.9
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG13	9	0.9
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	3	0.9
(1,916)	1:58:A:TYR:HB3	1:66:A:LYS:HB2	3	0.9
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	13	0.9
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	18	0.9
(1,873)	1:55:A:THR:H	1:55:A:THR:HG21	8	0.9
(1,873)	1:55:A:THR:H	1:55:A:THR:HG22	12	0.9
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	10	0.9
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	7	0.9
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	14	0.9
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	17	0.9
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	1	0.9
(1,817)	1:51:A:LEU:HB2	1:53:A:GLY:HA2	14	0.9
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	11	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB1	13	0.9
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB3	4	0.9
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB3	6	0.9
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	19	0.9
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	20	0.9
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	16	0.9
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	18	0.9
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	19	0.9
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	7	0.9
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	16	0.9
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	10	0.9
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	15	0.9
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	8	0.9
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	12	0.9
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	18	0.9
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	19	0.9
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	15	0.9
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	17	0.9
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	1	0.9
(1,183)	1:7:A:PRO:HG3	1:21:A:LYS:HG3	19	0.9
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	18	0.9
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	10	0.9
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	15	0.9
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	20	0.9
(1,1882)	1:2:A:VAL:H	1:2:A:VAL:HG13	19	0.89
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	18	0.89
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	3	0.89
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	15	0.89
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	7	0.89
(1,1500)	1:51:A:LEU:HD22	1:50:A:CYS:H	13	0.89
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	10	0.89
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	16	0.89
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	18	0.89
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	4	0.89
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	3	0.89
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	9	0.89
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	20	0.89
(1,1402)	1:80:A:LEU:HD23	1:75:A:GLY:HA3	17	0.89
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	18	0.89
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	1	0.89
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	8	0.89
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	11	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	12	0.89
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	14	0.89
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	8	0.89
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	20	0.89
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	18	0.89
(1,1292)	1:80:A:LEU:HA	1:79:A:GLN:HG3	1	0.89
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	19	0.89
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	14	0.89
(1,1182)	1:72:A:GLY:HA2	1:71:A:TYR:HD1	13	0.89
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	11	0.89
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	12	0.89
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	1	0.89
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	5	0.89
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	8	0.89
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	8	0.89
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	16	0.89
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	6	0.89
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG22	4	0.89
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG22	7	0.89
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	11	0.89
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	7	0.89
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	1	0.89
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	19	0.89
(1,943)	1:59:A:VAL:HG13	1:65:A:TYR:HB3	12	0.89
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	7	0.89
(1,873)	1:55:A:THR:H	1:55:A:THR:HG23	5	0.89
(1,873)	1:55:A:THR:H	1:55:A:THR:HG23	20	0.89
(1,872)	1:55:A:THR:HG21	1:67:A:CYS:HA	18	0.89
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	19	0.89
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	4	0.89
(1,820)	1:51:A:LEU:HB2	1:51:A:LEU:HD21	3	0.89
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	1	0.89
(1,703)	1:44:A:ALA:HB1	1:58:A:TYR:HA	5	0.89
(1,703)	1:44:A:ALA:HB2	1:58:A:TYR:HA	13	0.89
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB1	8	0.89
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	10	0.89
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	17	0.89
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	20	0.89
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG21	10	0.89
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	14	0.89
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	19	0.89
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	3	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	13	0.89
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	11	0.89
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	16	0.89
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	5	0.89
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG11	2	0.89
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	10	0.89
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	4	0.89
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	3	0.89
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	13	0.89
(1,401)	1:23:A:GLY:HA3	1:24:A:LEU:HD23	14	0.89
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	4	0.89
(1,302)	1:18:A:THR:HG21	1:20:A:LYS:HD2	5	0.89
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	8	0.89
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	9	0.89
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	12	0.89
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	15	0.89
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	17	0.89
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	11	0.89
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	4	0.89
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	8	0.89
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	18	0.89
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	20	0.89
(1,9)	1:31:A:CYS:HB2	1:32:A:ARG:HG2	20	0.89
(1,1882)	1:2:A:VAL:H	1:2:A:VAL:HG11	4	0.88
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	18	0.88
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	12	0.88
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	6	0.88
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD23	13	0.88
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	3	0.88
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	3	0.88
(1,1500)	1:51:A:LEU:HD21	1:50:A:CYS:H	18	0.88
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	5	0.88
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	4	0.88
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	3	0.88
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	12	0.88
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	15	0.88
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	12	0.88
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	15	0.88
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	16	0.88
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	1	0.88
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	8	0.88
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	18	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	17	0.88
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	16	0.88
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	3	0.88
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	4	0.88
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	6	0.88
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	13	0.88
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	16	0.88
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	19	0.88
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	7	0.88
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	20	0.88
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	18	0.88
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	8	0.88
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	19	0.88
(1,1319)	1:79:A:GLN:HG3	1:80:A:LEU:HD21	7	0.88
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD13	2	0.88
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	6	0.88
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	17	0.88
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	4	0.88
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	6	0.88
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	13	0.88
(1,1161)	1:71:A:TYR:HA	1:72:A:GLY:HA3	4	0.88
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	15	0.88
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	14	0.88
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	5	0.88
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	8	0.88
(1,1103)	1:69:A:CYS:HB2	1:78:A:CYS:HA	11	0.88
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	15	0.88
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	5	0.88
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	10	0.88
(1,988)	1:62:A:TYR:HA	1:62:A:TYR:HD1	8	0.88
(1,965)	1:59:A:VAL:HG22	1:64:A:TYR:H	1	0.88
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG11	18	0.88
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG12	18	0.88
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	4	0.88
(1,873)	1:55:A:THR:H	1:55:A:THR:HG21	7	0.88
(1,873)	1:55:A:THR:H	1:55:A:THR:HG23	11	0.88
(1,869)	1:55:A:THR:HG21	1:68:A:SER:HB3	5	0.88
(1,827)	1:51:A:LEU:HD11	1:51:A:LEU:H	20	0.88
(1,787)	1:49:A:PRO:HD3	1:48:A:ASN:HB3	1	0.88
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	13	0.88
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	16	0.88
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	10	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	1	0.88
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	11	0.88
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG22	15	0.88
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	7	0.88
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	12	0.88
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	8	0.88
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	7	0.88
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	18	0.88
(1,412)	1:24:A:LEU:H	1:24:A:LEU:HD23	14	0.88
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	6	0.88
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	13	0.88
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	4	0.88
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	8	0.88
(1,256)	1:14:A:ARG:HD2	1:14:A:ARG:H	1	0.88
(1,183)	1:7:A:PRO:HG3	1:21:A:LYS:HG3	6	0.88
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	14	0.88
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG23	16	0.88
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	6	0.88
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	12	0.88
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	12	0.88
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	4	0.88
(1,20)	1:56:A:CYS:H	1:67:A:CYS:HA	14	0.88
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	12	0.88
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE3	14	0.88
(1,1882)	1:2:A:VAL:H	1:2:A:VAL:HG11	11	0.87
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	3	0.87
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	12	0.87
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	19	0.87
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	9	0.87
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	3	0.87
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	4	0.87
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	10	0.87
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	19	0.87
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	17	0.87
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	14	0.87
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	7	0.87
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	16	0.87
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	19	0.87
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	14	0.87
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	14	0.87
(1,1415)	1:66:A:LYS:HB3	1:66:A:LYS:HE2	1	0.87
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	19	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	9	0.87
(1,1389)	1:83:A:TYR:HA	1:82:A:LYS:HA	15	0.87
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	15	0.87
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	2	0.87
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	7	0.87
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	20	0.87
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD21	1	0.87
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD23	11	0.87
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD11	16	0.87
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD11	20	0.87
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	18	0.87
(1,1279)	1:79:A:GLN:HB2	1:77:A:GLN:H	18	0.87
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD23	1	0.87
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	1	0.87
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	9	0.87
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	12	0.87
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	1	0.87
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	20	0.87
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	19	0.87
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	9	0.87
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	4	0.87
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	18	0.87
(1,953)	1:59:A:VAL:HG13	1:60:A:TYR:HD1	20	0.87
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG11	11	0.87
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	13	0.87
(1,873)	1:55:A:THR:H	1:55:A:THR:HG22	17	0.87
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	16	0.87
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	18	0.87
(1,822)	1:51:A:LEU:HD21	1:56:A:CYS:HB3	12	0.87
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	3	0.87
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	4	0.87
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	14	0.87
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	20	0.87
(1,707)	1:44:A:ALA:HB3	1:58:A:TYR:HD1	10	0.87
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB2	5	0.87
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	13	0.87
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	4	0.87
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	8	0.87
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG22	16	0.87
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	19	0.87
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	19	0.87
(1,510)	1:31:A:CYS:HB2	1:40:A:CYS:HB2	20	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	5	0.87
(1,437)	1:25:A:TYR:HB2	1:26:A:SER:HB2	6	0.87
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	12	0.87
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	4	0.87
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	9	0.87
(1,305)	1:18:A:THR:HG23	1:17:A:GLY:HA2	10	0.87
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	10	0.87
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	8	0.87
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	5	0.87
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	8	0.87
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	3	0.87
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	7	0.87
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	8	0.87
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	15	0.87
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	18	0.87
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	9	0.87
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	14	0.87
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	18	0.87
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	20	0.87
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	7	0.87
(1,24)	1:78:A:CYS:HB3	1:70:A:PRO:HD3	20	0.87
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	10	0.87
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	11	0.87
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	13	0.87
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	17	0.87
(1,1882)	1:2:A:VAL:H	1:2:A:VAL:HG13	8	0.86
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	11	0.86
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	6	0.86
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	9	0.86
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	9	0.86
(1,1634)	1:34:A:GLY:H	1:33:A:LYS:HG2	8	0.86
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	2	0.86
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	3	0.86
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	11	0.86
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	11	0.86
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	20	0.86
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	19	0.86
(1,1402)	1:80:A:LEU:HD23	1:75:A:GLY:HA3	1	0.86
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	16	0.86
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	9	0.86
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	6	0.86
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	9	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	14	0.86
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	12	0.86
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	18	0.86
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	10	0.86
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD13	4	0.86
(1,1314)	1:81:A:LYS:H	1:80:A:LEU:HD11	10	0.86
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	8	0.86
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD13	13	0.86
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	9	0.86
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	12	0.86
(1,1255)	1:78:A:CYS:HB3	1:51:A:LEU:HB3	13	0.86
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD12	10	0.86
(1,1207)	1:75:A:GLY:HA2	1:76:A:LYS:HG3	12	0.86
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	7	0.86
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	19	0.86
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	14	0.86
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	17	0.86
(1,1102)	1:69:A:CYS:HB3	1:68:A:SER:HB3	13	0.86
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	14	0.86
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	4	0.86
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	5	0.86
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	11	0.86
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	11	0.86
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	12	0.86
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	19	0.86
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	8	0.86
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	14	0.86
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	3	0.86
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	6	0.86
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	7	0.86
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	9	0.86
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	12	0.86
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	15	0.86
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	17	0.86
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	18	0.86
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	6	0.86
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	8	0.86
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB1	14	0.86
(1,698)	1:44:A:ALA:HB1	1:65:A:TYR:HB2	13	0.86
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	12	0.86
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	1	0.86
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	12	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	6	0.86
(1,641)	1:39:A:ASN:HA	1:29:A:CYS:HB3	3	0.86
(1,617)	1:38:A:LYS:HA	1:38:A:LYS:HE3	13	0.86
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	19	0.86
(1,607)	1:36:A:THR:H	1:36:A:THR:HG22	16	0.86
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	3	0.86
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	16	0.86
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	2	0.86
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	4	0.86
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	3	0.86
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG12	5	0.86
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	15	0.86
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	16	0.86
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	20	0.86
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	6	0.86
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	6	0.86
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	14	0.86
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	2	0.86
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	16	0.86
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	8	0.86
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	14	0.86
(1,305)	1:18:A:THR:HG21	1:17:A:GLY:HA2	7	0.86
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	9	0.86
(1,271)	1:17:A:GLY:HA2	1:13:A:CYS:HB2	20	0.86
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	10	0.86
(1,256)	1:14:A:ARG:HD2	1:14:A:ARG:H	5	0.86
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	2	0.86
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	1	0.86
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	1	0.86
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	3	0.86
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	7	0.86
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	8	0.86
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	13	0.86
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG22	18	0.86
(1,93)	1:3:A:TYR:HB3	1:3:A:TYR:HD1	17	0.86
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	6	0.86
(1,9)	1:31:A:CYS:HB2	1:32:A:ARG:HG2	5	0.86
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	11	0.86
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	14	0.86
(1,1882)	1:2:A:VAL:H	1:2:A:VAL:HG11	1	0.85
(1,1882)	1:2:A:VAL:H	1:2:A:VAL:HG11	2	0.85
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	15	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	14	0.85
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	18	0.85
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	15	0.85
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	9	0.85
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	17	0.85
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	8	0.85
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	4	0.85
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	8	0.85
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	8	0.85
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	20	0.85
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	1	0.85
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	4	0.85
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	6	0.85
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	8	0.85
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	14	0.85
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	13	0.85
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	17	0.85
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	4	0.85
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	9	0.85
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	17	0.85
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	3	0.85
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	1	0.85
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	12	0.85
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	2	0.85
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	11	0.85
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	13	0.85
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	20	0.85
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	9	0.85
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	8	0.85
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	8	0.85
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	15	0.85
(1,943)	1:59:A:VAL:HG12	1:65:A:TYR:HB3	18	0.85
(1,940)	1:59:A:VAL:HG11	1:66:A:LYS:HG2	8	0.85
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	9	0.85
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	6	0.85
(1,865)	1:55:A:THR:HG23	1:56:A:CYS:HB3	13	0.85
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	9	0.85
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	4	0.85
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	6	0.85
(1,822)	1:51:A:LEU:HD21	1:56:A:CYS:HB3	7	0.85
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	1	0.85
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	8	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	10	0.85
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	16	0.85
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	19	0.85
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB1	17	0.85
(1,706)	1:44:A:ALA:HB1	1:64:A:TYR:HD1	12	0.85
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	12	0.85
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	19	0.85
(1,653)	1:39:A:ASN:HA	1:40:A:CYS:HA	7	0.85
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	5	0.85
(1,564)	1:34:A:GLY:HA3	1:58:A:TYR:HE1	17	0.85
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	1	0.85
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	5	0.85
(1,529)	1:16:A:GLY:HA2	1:32:A:ARG:HD2	9	0.85
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	10	0.85
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	14	0.85
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	10	0.85
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	5	0.85
(1,262)	1:15:A:ASN:HB3	1:35:A:TYR:HD1	12	0.85
(1,256)	1:14:A:ARG:HD2	1:14:A:ARG:H	19	0.85
(1,235)	1:11:A:TYR:HA	1:11:A:TYR:HD1	20	0.85
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	7	0.85
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	4	0.85
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	6	0.85
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	10	0.85
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	10	0.85
(1,131)	1:5:A:PRO:HD3	1:4:A:TYR:HB2	16	0.85
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	16	0.85
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	5	0.85
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	3	0.85
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	7	0.85
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	9	0.85
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	7	0.85
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	14	0.85
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	4	0.84
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD22	11	0.84
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	7	0.84
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	12	0.84
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	13	0.84
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	9	0.84
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	13	0.84
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	14	0.84
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	7	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	19	0.84
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	11	0.84
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	10	0.84
(1,1398)	1:78:A:CYS:HA	1:69:A:CYS:HB3	4	0.84
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	11	0.84
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	7	0.84
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	12	0.84
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	17	0.84
(1,1316)	1:80:A:LEU:HD22	1:80:A:LEU:HB2	15	0.84
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	17	0.84
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	5	0.84
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	20	0.84
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	14	0.84
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	5	0.84
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	9	0.84
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	9	0.84
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	12	0.84
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	16	0.84
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	8	0.84
(1,866)	1:55:A:THR:HG21	1:56:A:CYS:HB2	6	0.84
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	12	0.84
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	12	0.84
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	2	0.84
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	5	0.84
(1,746)	1:47:A:PRO:HB3	1:47:A:PRO:HD2	13	0.84
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	3	0.84
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	19	0.84
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB3	12	0.84
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB3	11	0.84
(1,697)	1:44:A:ALA:HB3	1:34:A:GLY:HA2	8	0.84
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	17	0.84
(1,607)	1:36:A:THR:H	1:36:A:THR:HG23	9	0.84
(1,607)	1:36:A:THR:H	1:36:A:THR:HG23	12	0.84
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	11	0.84
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	18	0.84
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	11	0.84
(1,483)	1:28:A:LYS:HB3	1:28:A:LYS:HE2	18	0.84
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	18	0.84
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	11	0.84
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	8	0.84
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	9	0.84
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD22	3	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:22:A:ARG:HG3	1:28:A:LYS:H	7	0.84
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	11	0.84
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	5	0.84
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	19	0.84
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	12	0.84
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	7	0.84
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	11	0.84
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	6	0.84
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	18	0.84
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	7	0.84
(1,166)	1:7:A:PRO:HD3	1:21:A:LYS:HG3	11	0.84
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	7	0.84
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	20	0.84
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	15	0.84
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG21	20	0.84
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	6	0.84
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	20	0.84
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	3	0.84
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	16	0.84
(1,9)	1:31:A:CYS:HB2	1:32:A:ARG:HG2	7	0.84
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	19	0.84
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	18	0.83
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	12	0.83
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	15	0.83
(1,1402)	1:80:A:LEU:HD22	1:75:A:GLY:HA3	11	0.83
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	11	0.83
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	6	0.83
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	4	0.83
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	17	0.83
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	12	0.83
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	14	0.83
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	4	0.83
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	7	0.83
(1,1316)	1:80:A:LEU:HD22	1:80:A:LEU:HB2	3	0.83
(1,1316)	1:80:A:LEU:HD22	1:80:A:LEU:HB2	4	0.83
(1,1316)	1:80:A:LEU:HD23	1:80:A:LEU:HB2	5	0.83
(1,1316)	1:80:A:LEU:HD22	1:80:A:LEU:HB2	9	0.83
(1,1316)	1:80:A:LEU:HD22	1:80:A:LEU:HB2	12	0.83
(1,1316)	1:80:A:LEU:HD21	1:80:A:LEU:HB2	13	0.83
(1,1316)	1:80:A:LEU:HD21	1:80:A:LEU:HB2	16	0.83
(1,1316)	1:80:A:LEU:HD21	1:80:A:LEU:HB2	20	0.83
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD13	11	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD13	15	0.83
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD11	7	0.83
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	4	0.83
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	4	0.83
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	9	0.83
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	4	0.83
(1,1207)	1:75:A:GLY:HA2	1:76:A:LYS:HG3	4	0.83
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	15	0.83
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	19	0.83
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	14	0.83
(1,1103)	1:69:A:CYS:HB2	1:78:A:CYS:HA	4	0.83
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	9	0.83
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	13	0.83
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	10	0.83
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	8	0.83
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	7	0.83
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG11	1	0.83
(1,940)	1:59:A:VAL:HG13	1:66:A:LYS:HG2	6	0.83
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	12	0.83
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	8	0.83
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	13	0.83
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	14	0.83
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	17	0.83
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	11	0.83
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	19	0.83
(1,695)	1:44:A:ALA:HB1	1:45:A:CYS:HB3	7	0.83
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	6	0.83
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	9	0.83
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	9	0.83
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	8	0.83
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	20	0.83
(1,483)	1:28:A:LYS:HB3	1:28:A:LYS:HE2	1	0.83
(1,483)	1:28:A:LYS:HB3	1:28:A:LYS:HE2	19	0.83
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	19	0.83
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	20	0.83
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	17	0.83
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	4	0.83
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	7	0.83
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	9	0.83
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	10	0.83
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	7	0.83
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	19	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:18:A:THR:HG22	1:17:A:GLY:HA2	12	0.83
(1,305)	1:18:A:THR:HG22	1:17:A:GLY:HA2	20	0.83
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	18	0.83
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	6	0.83
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	7	0.83
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	3	0.83
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	6	0.83
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	16	0.83
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	20	0.83
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG22	3	0.83
(1,96)	1:3:A:TYR:HB2	1:3:A:TYR:H	17	0.83
(1,84)	1:3:A:TYR:H	1:2:A:VAL:HG21	11	0.83
(1,61)	1:71:A:TYR:HE1	1:71:A:TYR:HA	3	0.83
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	1	0.83
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	18	0.83
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	8	0.82
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	19	0.82
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	15	0.82
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD22	15	0.82
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	14	0.82
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	4	0.82
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	12	0.82
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	6	0.82
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	8	0.82
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	5	0.82
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	17	0.82
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	5	0.82
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	16	0.82
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	18	0.82
(1,1316)	1:80:A:LEU:HD21	1:80:A:LEU:HB2	1	0.82
(1,1316)	1:80:A:LEU:HD22	1:80:A:LEU:HB2	6	0.82
(1,1316)	1:80:A:LEU:HD21	1:80:A:LEU:HB2	8	0.82
(1,1316)	1:80:A:LEU:HD21	1:80:A:LEU:HB2	10	0.82
(1,1316)	1:80:A:LEU:HD23	1:80:A:LEU:HB2	11	0.82
(1,1316)	1:80:A:LEU:HD22	1:80:A:LEU:HB2	14	0.82
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	9	0.82
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	18	0.82
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	19	0.82
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	5	0.82
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	2	0.82
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	11	0.82
(1,1166)	1:71:A:TYR:HA	1:71:A:TYR:HD1	5	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	17	0.82
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	3	0.82
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	6	0.82
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	18	0.82
(1,1036)	1:59:A:VAL:HG11	1:65:A:TYR:HA	14	0.82
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	1	0.82
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG11	6	0.82
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG11	10	0.82
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG11	20	0.82
(1,865)	1:55:A:THR:HG22	1:56:A:CYS:HB3	17	0.82
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	5	0.82
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	13	0.82
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	15	0.82
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	6	0.82
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	8	0.82
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	10	0.82
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	18	0.82
(1,703)	1:44:A:ALA:HB3	1:58:A:TYR:HA	12	0.82
(1,699)	1:44:A:ALA:HB1	1:64:A:TYR:HB3	3	0.82
(1,695)	1:44:A:ALA:HB3	1:45:A:CYS:HB3	18	0.82
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	2	0.82
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG23	5	0.82
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	14	0.82
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	18	0.82
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	1	0.82
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	2	0.82
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	20	0.82
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	6	0.82
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	11	0.82
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	18	0.82
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	19	0.82
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	13	0.82
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	9	0.82
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	13	0.82
(1,256)	1:14:A:ARG:HD2	1:14:A:ARG:H	3	0.82
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	7	0.82
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	5	0.82
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	20	0.82
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	5	0.82
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	13	0.82
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	5	0.82
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	14	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	16	0.82
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	5	0.82
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	15	0.82
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	4	0.82
(1,61)	1:71:A:TYR:HE1	1:71:A:TYR:HA	19	0.82
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	9	0.82
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	9	0.82
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	4	0.81
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	5	0.81
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	5	0.81
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	4	0.81
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	12	0.81
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	19	0.81
(1,1488)	1:4:A:TYR:HB2	1:3:A:TYR:HA	6	0.81
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	2	0.81
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	14	0.81
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	19	0.81
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	9	0.81
(1,1418)	1:62:A:TYR:HB3	1:62:A:TYR:HD1	8	0.81
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	14	0.81
(1,1402)	1:80:A:LEU:HD23	1:75:A:GLY:HA3	18	0.81
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	20	0.81
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD21	12	0.81
(1,1316)	1:80:A:LEU:HD22	1:80:A:LEU:HB2	7	0.81
(1,1316)	1:80:A:LEU:HD21	1:80:A:LEU:HB2	17	0.81
(1,1316)	1:80:A:LEU:HD21	1:80:A:LEU:HB2	18	0.81
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	5	0.81
(1,1313)	1:75:A:GLY:H	1:80:A:LEU:HD12	14	0.81
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	5	0.81
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	20	0.81
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	18	0.81
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	9	0.81
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	17	0.81
(1,1115)	1:71:A:TYR:HB2	1:70:A:PRO:HA	9	0.81
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	14	0.81
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG21	5	0.81
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	13	0.81
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	3	0.81
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	15	0.81
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG12	7	0.81
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG11	18	0.81
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG11	20	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	1	0.81
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	15	0.81
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	18	0.81
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	1	0.81
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	18	0.81
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	1	0.81
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	8	0.81
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	10	0.81
(1,827)	1:51:A:LEU:HD13	1:51:A:LEU:H	14	0.81
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	8	0.81
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	14	0.81
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	11	0.81
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	7	0.81
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB3	10	0.81
(1,698)	1:44:A:ALA:HB3	1:65:A:TYR:HB2	5	0.81
(1,695)	1:44:A:ALA:HB3	1:45:A:CYS:HB3	14	0.81
(1,633)	1:66:A:LYS:HE2	1:66:A:LYS:HG3	6	0.81
(1,607)	1:36:A:THR:H	1:36:A:THR:HG22	6	0.81
(1,607)	1:36:A:THR:H	1:36:A:THR:HG23	20	0.81
(1,599)	1:36:A:THR:HG21	1:64:A:TYR:HB3	19	0.81
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG22	6	0.81
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	8	0.81
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	7	0.81
(1,483)	1:28:A:LYS:HB3	1:28:A:LYS:HE2	14	0.81
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG11	16	0.81
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	5	0.81
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	16	0.81
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	2	0.81
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	5	0.81
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	11	0.81
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	19	0.81
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	7	0.81
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	12	0.81
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	20	0.81
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	12	0.81
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	15	0.81
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	2	0.81
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	9	0.81
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	7	0.81
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	9	0.81
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	17	0.81
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	14	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	4	0.81
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	8	0.81
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	12	0.81
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	8	0.81
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG21	17	0.81
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	12	0.81
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	5	0.81
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	6	0.81
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	17	0.81
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	19	0.81
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	17	0.81
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	15	0.81
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	8	0.8
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	14	0.8
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	20	0.8
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	14	0.8
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	13	0.8
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	3	0.8
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	7	0.8
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	20	0.8
(1,1402)	1:80:A:LEU:HD22	1:75:A:GLY:HA3	5	0.8
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	1	0.8
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	2	0.8
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	14	0.8
(1,1322)	1:81:A:LYS:H	1:80:A:LEU:HD22	9	0.8
(1,1316)	1:80:A:LEU:HD22	1:80:A:LEU:HB2	2	0.8
(1,1316)	1:80:A:LEU:HD23	1:80:A:LEU:HB2	19	0.8
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	19	0.8
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	19	0.8
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	9	0.8
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	15	0.8
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	10	0.8
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	6	0.8
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	20	0.8
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	1	0.8
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	9	0.8
(1,1207)	1:75:A:GLY:HA2	1:76:A:LYS:HG3	1	0.8
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	7	0.8
(1,1166)	1:71:A:TYR:HA	1:71:A:TYR:HD1	6	0.8
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	18	0.8
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	6	0.8
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	3	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	4	0.8
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	17	0.8
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	10	0.8
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	13	0.8
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG13	4	0.8
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG11	9	0.8
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG13	19	0.8
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG13	4	0.8
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	10	0.8
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	6	0.8
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	1	0.8
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	10	0.8
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	16	0.8
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	6	0.8
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	7	0.8
(1,822)	1:51:A:LEU:HD21	1:56:A:CYS:HB3	2	0.8
(1,822)	1:51:A:LEU:HD22	1:56:A:CYS:HB3	5	0.8
(1,787)	1:49:A:PRO:HD3	1:48:A:ASN:HB3	12	0.8
(1,787)	1:49:A:PRO:HD3	1:48:A:ASN:HB3	20	0.8
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	19	0.8
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	17	0.8
(1,703)	1:44:A:ALA:HB1	1:58:A:TYR:HA	16	0.8
(1,703)	1:44:A:ALA:HB3	1:58:A:TYR:HA	17	0.8
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB3	15	0.8
(1,697)	1:44:A:ALA:HB3	1:34:A:GLY:HA2	3	0.8
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	3	0.8
(1,662)	1:40:A:CYS:HB2	1:32:A:ARG:HA	7	0.8
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	14	0.8
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	18	0.8
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG23	9	0.8
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG12	10	0.8
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	4	0.8
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	13	0.8
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	3	0.8
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	16	0.8
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	1	0.8
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	11	0.8
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	10	0.8
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	18	0.8
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	1	0.8
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	4	0.8
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	5	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	10	0.8
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	15	0.8
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	3	0.8
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	1	0.8
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	3	0.8
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	4	0.8
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	6	0.8
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	19	0.8
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	17	0.8
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	12	0.8
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	14	0.8
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	4	0.8
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	15	0.8
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	17	0.8
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	2	0.8
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	10	0.8
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	17	0.8
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG22	5	0.8
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	4	0.8
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	2	0.8
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	11	0.8
(1,84)	1:3:A:TYR:H	1:2:A:VAL:HG21	12	0.8
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	2	0.8
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	3	0.8
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	2	0.79
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	18	0.79
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	9	0.79
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	15	0.79
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	12	0.79
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	5	0.79
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	6	0.79
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	19	0.79
(1,1672)	1:79:A:GLN:H	1:77:A:GLN:HB2	14	0.79
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	10	0.79
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD23	20	0.79
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	5	0.79
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	13	0.79
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	15	0.79
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	4	0.79
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	4	0.79
(1,1467)	1:22:A:ARG:HD2	1:22:A:ARG:H	3	0.79
(1,1467)	1:22:A:ARG:HD2	1:22:A:ARG:H	17	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	19	0.79
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	10	0.79
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	7	0.79
(1,1384)	1:83:A:TYR:HA	1:81:A:LYS:HG3	3	0.79
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	7	0.79
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	19	0.79
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	12	0.79
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	6	0.79
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	16	0.79
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	9	0.79
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	13	0.79
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	15	0.79
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	12	0.79
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	18	0.79
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	19	0.79
(1,1064)	1:66:A:LYS:HG3	1:59:A:VAL:HG23	1	0.79
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	17	0.79
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	15	0.79
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	12	0.79
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	18	0.79
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	11	0.79
(1,960)	1:59:A:VAL:HG23	1:60:A:TYR:HB2	20	0.79
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG12	3	0.79
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG13	12	0.79
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG12	13	0.79
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG11	17	0.79
(1,940)	1:59:A:VAL:HG11	1:66:A:LYS:HG2	3	0.79
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	17	0.79
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	3	0.79
(1,827)	1:51:A:LEU:HD13	1:51:A:LEU:H	10	0.79
(1,824)	1:51:A:LEU:HD22	1:51:A:LEU:H	2	0.79
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	9	0.79
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	18	0.79
(1,797)	1:50:A:CYS:HA	1:78:A:CYS:HB2	12	0.79
(1,794)	1:50:A:CYS:HA	1:77:A:GLN:HG2	5	0.79
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	17	0.79
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	17	0.79
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	13	0.79
(1,703)	1:44:A:ALA:HB1	1:58:A:TYR:HA	7	0.79
(1,698)	1:44:A:ALA:HB1	1:65:A:TYR:HB2	6	0.79
(1,695)	1:44:A:ALA:HB2	1:45:A:CYS:HB3	19	0.79
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	4	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	7	0.79
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	14	0.79
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	8	0.79
(1,624)	1:38:A:LYS:HB3	1:37:A:GLY:HA2	13	0.79
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG23	4	0.79
(1,607)	1:36:A:THR:H	1:36:A:THR:HG21	10	0.79
(1,607)	1:36:A:THR:H	1:36:A:THR:HG22	15	0.79
(1,607)	1:36:A:THR:H	1:36:A:THR:HG21	18	0.79
(1,607)	1:36:A:THR:H	1:36:A:THR:HG23	19	0.79
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	6	0.79
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	19	0.79
(1,542)	1:33:A:LYS:HA	1:34:A:GLY:HA2	8	0.79
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	12	0.79
(1,483)	1:28:A:LYS:HB3	1:28:A:LYS:HE2	7	0.79
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG11	9	0.79
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	13	0.79
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	19	0.79
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	5	0.79
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	13	0.79
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	2	0.79
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	3	0.79
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	8	0.79
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	9	0.79
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	14	0.79
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	17	0.79
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	16	0.79
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	8	0.79
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	9	0.79
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	18	0.79
(1,302)	1:18:A:THR:HG21	1:20:A:LYS:HD2	6	0.79
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	1	0.79
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	4	0.79
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	19	0.79
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	15	0.79
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	14	0.79
(1,216)	1:10:A:PRO:HB2	1:10:A:PRO:HD2	2	0.79
(1,216)	1:10:A:PRO:HB2	1:10:A:PRO:HD2	11	0.79
(1,216)	1:10:A:PRO:HB2	1:10:A:PRO:HD2	13	0.79
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	6	0.79
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	14	0.79
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	15	0.79
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	13	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	16	0.79
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	12	0.79
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	16	0.79
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	9	0.79
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	5	0.79
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	16	0.79
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	5	0.79
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	19	0.79
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	13	0.78
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	17	0.78
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	11	0.78
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	1	0.78
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	4	0.78
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	3	0.78
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD11	11	0.78
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	8	0.78
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	15	0.78
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	19	0.78
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	11	0.78
(1,1478)	1:18:A:THR:HG22	1:20:A:LYS:HB3	11	0.78
(1,1478)	1:18:A:THR:HG22	1:20:A:LYS:HB3	14	0.78
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	4	0.78
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	16	0.78
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	12	0.78
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	14	0.78
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	4	0.78
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	7	0.78
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	12	0.78
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	1	0.78
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	15	0.78
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	16	0.78
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD23	17	0.78
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	2	0.78
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	5	0.78
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	10	0.78
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	17	0.78
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	1	0.78
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	2	0.78
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	3	0.78
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	8	0.78
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	11	0.78
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	20	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	12	0.78
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	2	0.78
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	13	0.78
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	17	0.78
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	18	0.78
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	10	0.78
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	18	0.78
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	11	0.78
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	19	0.78
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	2	0.78
(1,1037)	1:65:A:TYR:HA	1:66:A:LYS:HB2	15	0.78
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	2	0.78
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	11	0.78
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	13	0.78
(1,978)	1:60:A:TYR:H	1:60:A:TYR:HB2	9	0.78
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	2	0.78
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	20	0.78
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG13	9	0.78
(1,952)	1:59:A:VAL:HG11	1:58:A:TYR:HD1	9	0.78
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG13	2	0.78
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG11	5	0.78
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG12	8	0.78
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG13	16	0.78
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	1	0.78
(1,865)	1:55:A:THR:HG22	1:56:A:CYS:HB3	3	0.78
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	14	0.78
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	2	0.78
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	6	0.78
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	7	0.78
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	9	0.78
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	20	0.78
(1,827)	1:51:A:LEU:HD11	1:51:A:LEU:H	11	0.78
(1,824)	1:51:A:LEU:HD23	1:51:A:LEU:H	3	0.78
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	5	0.78
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	8	0.78
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	11	0.78
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	14	0.78
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	17	0.78
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	10	0.78
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	20	0.78
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	3	0.78
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	8	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB3	2	0.78
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	19	0.78
(1,633)	1:66:A:LYS:HE2	1:66:A:LYS:HG3	8	0.78
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	12	0.78
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	17	0.78
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG21	11	0.78
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG22	14	0.78
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG23	1	0.78
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	11	0.78
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	1	0.78
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	3	0.78
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	4	0.78
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	13	0.78
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	17	0.78
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	19	0.78
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	13	0.78
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	18	0.78
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	17	0.78
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG22	2	0.78
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	3	0.78
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	1	0.78
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	16	0.78
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	8	0.78
(1,216)	1:10:A:PRO:HB2	1:10:A:PRO:HD2	10	0.78
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	8	0.78
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	1	0.78
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	1	0.78
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	11	0.78
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	13	0.78
(1,77)	1:2:A:VAL:HB	1:4:A:TYR:HE1	15	0.78
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	11	0.78
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	12	0.78
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	14	0.78
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	1	0.78
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	4	0.78
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	15	0.78
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	2	0.78
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	9	0.78
(1,6)	1:7:A:PRO:HD2	1:27:A:TYR:HB2	15	0.78
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	7	0.77
(1,1785)	1:67:A:CYS:H	1:66:A:LYS:HB3	20	0.77
(1,1671)	1:41:A:GLN:H	1:39:A:ASN:HB3	14	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1645)	1:35:A:TYR:H	1:33:A:LYS:HG2	11	0.77
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	3	0.77
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	4	0.77
(1,1479)	1:14:A:ARG:HA	1:15:A:ASN:HA	4	0.77
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	10	0.77
(1,1418)	1:62:A:TYR:HB3	1:62:A:TYR:HD1	6	0.77
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	6	0.77
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	12	0.77
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	9	0.77
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	1	0.77
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	13	0.77
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD13	17	0.77
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	14	0.77
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	2	0.77
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	8	0.77
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	1	0.77
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	14	0.77
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	18	0.77
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	4	0.77
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	5	0.77
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	6	0.77
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	10	0.77
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	12	0.77
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	14	0.77
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	18	0.77
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	19	0.77
(1,1182)	1:72:A:GLY:HA2	1:71:A:TYR:HD1	15	0.77
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	19	0.77
(1,1166)	1:71:A:TYR:HA	1:71:A:TYR:HD1	10	0.77
(1,1166)	1:71:A:TYR:HA	1:71:A:TYR:HD1	11	0.77
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	20	0.77
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	10	0.77
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	10	0.77
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	5	0.77
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	7	0.77
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	10	0.77
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	20	0.77
(1,965)	1:59:A:VAL:HG23	1:64:A:TYR:H	6	0.77
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG12	15	0.77
(1,940)	1:59:A:VAL:HG13	1:66:A:LYS:HG2	18	0.77
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	7	0.77
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	5	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	1	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	1	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	2	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	4	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	6	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	7	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	10	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	12	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	13	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	15	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	16	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	19	0.77
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	20	0.77
(1,787)	1:49:A:PRO:HD3	1:48:A:ASN:HB3	3	0.77
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	1	0.77
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	12	0.77
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	11	0.77
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	14	0.77
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	15	0.77
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB2	3	0.77
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB1	16	0.77
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	6	0.77
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	15	0.77
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	19	0.77
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	11	0.77
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	19	0.77
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	6	0.77
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	15	0.77
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	9	0.77
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	3	0.77
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG11	1	0.77
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG13	15	0.77
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	9	0.77
(1,453)	1:22:A:ARG:HG2	1:27:A:TYR:HA	5	0.77
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	9	0.77
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	7	0.77
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	15	0.77
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	4	0.77
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	5	0.77
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	20	0.77
(1,216)	1:10:A:PRO:HB2	1:10:A:PRO:HD2	6	0.77
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	7	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:7:A:PRO:HG2	1:27:A:TYR:HA	16	0.77
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	8	0.77
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	9	0.77
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	18	0.77
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	3	0.77
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	9	0.77
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	3	0.77
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	18	0.77
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	20	0.77
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	15	0.77
(1,103)	1:4:A:TYR:HB2	1:4:A:TYR:HD1	10	0.77
(1,83)	1:2:A:VAL:HG22	1:4:A:TYR:HE1	19	0.77
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	8	0.77
(1,69)	1:20:A:LYS:HD3	1:30:A:TYR:HE1	17	0.77
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	7	0.77
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	2	0.77
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	11	0.77
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	14	0.76
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	2	0.76
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	9	0.76
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	5	0.76
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	17	0.76
(1,1478)	1:18:A:THR:HG22	1:20:A:LYS:HB3	3	0.76
(1,1478)	1:18:A:THR:HG21	1:20:A:LYS:HB3	6	0.76
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	11	0.76
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	18	0.76
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	2	0.76
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	3	0.76
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	7	0.76
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	17	0.76
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	17	0.76
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	18	0.76
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	2	0.76
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD11	11	0.76
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	2	0.76
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	6	0.76
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	3	0.76
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	4	0.76
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	19	0.76
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	4	0.76
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	16	0.76
(1,1196)	1:74:A:TYR:HB2	1:74:A:TYR:HE1	17	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	17	0.76
(1,1131)	1:70:A:PRO:HB3	1:73:A:TYR:HD1	3	0.76
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	9	0.76
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	11	0.76
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	2	0.76
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	5	0.76
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	9	0.76
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	19	0.76
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	20	0.76
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	2	0.76
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	10	0.76
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	20	0.76
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	2	0.76
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	3	0.76
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	4	0.76
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	20	0.76
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	1	0.76
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	16	0.76
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	8	0.76
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	12	0.76
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	18	0.76
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	12	0.76
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	17	0.76
(1,703)	1:44:A:ALA:HB2	1:58:A:TYR:HA	4	0.76
(1,698)	1:44:A:ALA:HB3	1:65:A:TYR:HB2	7	0.76
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	9	0.76
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	1	0.76
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	8	0.76
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	10	0.76
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	3	0.76
(1,614)	1:38:A:LYS:HA	1:38:A:LYS:HG2	9	0.76
(1,607)	1:36:A:THR:H	1:36:A:THR:HG22	14	0.76
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	12	0.76
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	4	0.76
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	11	0.76
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	13	0.76
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	8	0.76
(1,452)	1:22:A:ARG:HB3	1:27:A:TYR:HA	15	0.76
(1,433)	1:25:A:TYR:HB3	1:25:A:TYR:HE1	15	0.76
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	12	0.76
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	10	0.76
(1,297)	1:18:A:THR:HB	1:30:A:TYR:HE1	9	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	14	0.76
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	18	0.76
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	10	0.76
(1,216)	1:10:A:PRO:HB2	1:10:A:PRO:HD2	4	0.76
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	12	0.76
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	15	0.76
(1,179)	1:7:A:PRO:HG2	1:8:A:CYS:HA	13	0.76
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	7	0.76
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	8	0.76
(1,122)	1:5:A:PRO:HB3	1:3:A:TYR:HE1	12	0.76
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	18	0.76
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	20	0.76
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	18	0.76
(1,9)	1:31:A:CYS:HB2	1:32:A:ARG:HG2	2	0.76
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	6	0.76
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE2	17	0.76
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	5	0.75
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	13	0.75
(1,1821)	1:74:A:TYR:H	1:74:A:TYR:HE1	15	0.75
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	11	0.75
(1,1789)	1:67:A:CYS:H	1:65:A:TYR:HD1	9	0.75
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	5	0.75
(1,1698)	1:44:A:ALA:H	1:58:A:TYR:HE1	3	0.75
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	5	0.75
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	1	0.75
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	16	0.75
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	10	0.75
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	8	0.75
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	1	0.75
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	10	0.75
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	13	0.75
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	19	0.75
(1,1379)	1:82:A:LYS:HE2	1:74:A:TYR:HE1	5	0.75
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD22	19	0.75
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	13	0.75
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD21	16	0.75
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	7	0.75
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	3	0.75
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	7	0.75
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	12	0.75
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	12	0.75
(1,1046)	1:59:A:VAL:H	1:65:A:TYR:HA	9	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	19	0.75
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	3	0.75
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG13	11	0.75
(1,898)	1:57:A:GLY:HA3	1:58:A:TYR:HD1	2	0.75
(1,865)	1:55:A:THR:HG21	1:56:A:CYS:HB3	1	0.75
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	2	0.75
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	3	0.75
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	5	0.75
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	16	0.75
(1,854)	1:55:A:THR:HA	1:56:A:CYS:HB2	20	0.75
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	18	0.75
(1,828)	1:51:A:LEU:HD12	1:52:A:ASN:H	18	0.75
(1,827)	1:51:A:LEU:HD13	1:51:A:LEU:H	6	0.75
(1,808)	1:52:A:ASN:H	1:51:A:LEU:HA	3	0.75
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	17	0.75
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	7	0.75
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	12	0.75
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	11	0.75
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB2	16	0.75
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	7	0.75
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	20	0.75
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	13	0.75
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	5	0.75
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	18	0.75
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG21	2	0.75
(1,488)	1:28:A:LYS:HE2	1:28:A:LYS:HA	11	0.75
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG13	8	0.75
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	7	0.75
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	18	0.75
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	12	0.75
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	12	0.75
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	20	0.75
(1,314)	1:19:A:CYS:HB3	1:11:A:TYR:HE1	11	0.75
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	14	0.75
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	11	0.75
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	20	0.75
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	11	0.75
(1,216)	1:10:A:PRO:HB2	1:10:A:PRO:HD2	19	0.75
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	3	0.75
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	8	0.75
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	5	0.75
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	16	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	18	0.75
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	2	0.75
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	20	0.75
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	15	0.75
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	7	0.75
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	5	0.75
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	19	0.75
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	4	0.75
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	8	0.75
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	10	0.75
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	9	0.74
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	2	0.74
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	8	0.74
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	16	0.74
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	6	0.74
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	2	0.74
(1,1478)	1:18:A:THR:HG22	1:20:A:LYS:HB3	18	0.74
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	11	0.74
(1,1398)	1:78:A:CYS:HA	1:69:A:CYS:HB3	11	0.74
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	11	0.74
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	19	0.74
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	5	0.74
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD11	15	0.74
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	12	0.74
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	13	0.74
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	15	0.74
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	18	0.74
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	20	0.74
(1,1224)	1:76:A:LYS:HA	1:75:A:GLY:HA3	8	0.74
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	6	0.74
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	6	0.74
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	3	0.74
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	12	0.74
(1,1050)	1:65:A:TYR:HB3	1:58:A:TYR:HA	18	0.74
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	7	0.74
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	15	0.74
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	11	0.74
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	14	0.74
(1,949)	1:59:A:VAL:HA	1:59:A:VAL:HG13	14	0.74
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG13	19	0.74
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	11	0.74
(1,872)	1:55:A:THR:HG23	1:67:A:CYS:HA	5	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:55:A:THR:HG23	1:56:A:CYS:HB3	20	0.74
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	17	0.74
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	10	0.74
(1,787)	1:49:A:PRO:HD3	1:48:A:ASN:HB3	17	0.74
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	1	0.74
(1,739)	1:47:A:PRO:HA	1:48:A:ASN:HB2	10	0.74
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	9	0.74
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	20	0.74
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB2	9	0.74
(1,703)	1:44:A:ALA:HB3	1:58:A:TYR:HA	8	0.74
(1,698)	1:44:A:ALA:HB1	1:65:A:TYR:HB2	15	0.74
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	10	0.74
(1,599)	1:36:A:THR:HG23	1:64:A:TYR:HB3	4	0.74
(1,592)	1:36:A:THR:HB	1:44:A:ALA:HB2	2	0.74
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	11	0.74
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG23	20	0.74
(1,564)	1:34:A:GLY:HA3	1:58:A:TYR:HE1	11	0.74
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	12	0.74
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	6	0.74
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	12	0.74
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	14	0.74
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	14	0.74
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	1	0.74
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	15	0.74
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	10	0.74
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	13	0.74
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	17	0.74
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	10	0.74
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	11	0.74
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	1	0.74
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	19	0.74
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	19	0.74
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	3	0.74
(1,198)	1:9:A:SER:HB3	1:10:A:PRO:HA	20	0.74
(1,176)	1:7:A:PRO:HG2	1:21:A:LYS:HG3	20	0.74
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	14	0.74
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	6	0.74
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	12	0.74
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	3	0.74
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	10	0.74
(1,84)	1:3:A:TYR:H	1:2:A:VAL:HG21	19	0.74
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	19	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	10	0.73
(1,1857)	1:83:A:TYR:H	1:82:A:LYS:HG2	18	0.73
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	17	0.73
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	15	0.73
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	10	0.73
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	16	0.73
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	16	0.73
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	7	0.73
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	7	0.73
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	18	0.73
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	17	0.73
(1,1500)	1:51:A:LEU:HD23	1:50:A:CYS:H	15	0.73
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	8	0.73
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	4	0.73
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	10	0.73
(1,1382)	1:82:A:LYS:HG2	1:74:A:TYR:HD1	17	0.73
(1,1341)	1:81:A:LYS:HD2	1:83:A:TYR:HE1	7	0.73
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	2	0.73
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	13	0.73
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	14	0.73
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD13	18	0.73
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	6	0.73
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	17	0.73
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	15	0.73
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	20	0.73
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	6	0.73
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	7	0.73
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	15	0.73
(1,1166)	1:71:A:TYR:HA	1:71:A:TYR:HD1	7	0.73
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	15	0.73
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	11	0.73
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	4	0.73
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	15	0.73
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	6	0.73
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	11	0.73
(1,968)	1:60:A:TYR:HA	1:61:A:GLY:HA3	17	0.73
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	18	0.73
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	9	0.73
(1,827)	1:51:A:LEU:HD13	1:51:A:LEU:H	3	0.73
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	2	0.73
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	5	0.73
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	1	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,698)	1:44:A:ALA:HB1	1:65:A:TYR:HB2	11	0.73
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	13	0.73
(1,607)	1:36:A:THR:H	1:36:A:THR:HG23	5	0.73
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	18	0.73
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	20	0.73
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	11	0.73
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG12	18	0.73
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	15	0.73
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	8	0.73
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	9	0.73
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	10	0.73
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	14	0.73
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	2	0.73
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	7	0.73
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	17	0.73
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	10	0.73
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	10	0.73
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	6	0.73
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	19	0.73
(1,103)	1:4:A:TYR:HB2	1:4:A:TYR:HD1	13	0.73
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	6	0.73
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	13	0.73
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	4	0.73
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	15	0.73
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	13	0.73
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	6	0.73
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	14	0.73
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	8	0.73
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	15	0.73
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	3	0.72
(1,1800)	1:72:A:GLY:H	1:82:A:LYS:HB3	15	0.72
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	4	0.72
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	8	0.72
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	4	0.72
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	9	0.72
(1,1500)	1:51:A:LEU:HD21	1:50:A:CYS:H	5	0.72
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	18	0.72
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	2	0.72
(1,1410)	1:70:A:PRO:HG2	1:54:A:GLY:H	12	0.72
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	6	0.72
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	11	0.72
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	17	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	18	0.72
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	10	0.72
(1,1320)	1:79:A:GLN:HG2	1:80:A:LEU:HD21	4	0.72
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	17	0.72
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	11	0.72
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	3	0.72
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	6	0.72
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	16	0.72
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	8	0.72
(1,1185)	1:72:A:GLY:HA3	1:71:A:TYR:HD1	12	0.72
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	13	0.72
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	6	0.72
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	11	0.72
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	16	0.72
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	4	0.72
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	13	0.72
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	16	0.72
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	19	0.72
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	6	0.72
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	15	0.72
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	4	0.72
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	10	0.72
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG12	3	0.72
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG12	4	0.72
(1,872)	1:55:A:THR:HG23	1:67:A:CYS:HA	13	0.72
(1,865)	1:55:A:THR:HG23	1:56:A:CYS:HB3	5	0.72
(1,827)	1:51:A:LEU:HD13	1:51:A:LEU:H	1	0.72
(1,824)	1:51:A:LEU:HD22	1:51:A:LEU:H	7	0.72
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	15	0.72
(1,705)	1:44:A:ALA:HB2	1:65:A:TYR:HA	10	0.72
(1,663)	1:40:A:CYS:HB3	1:32:A:ARG:HA	7	0.72
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	15	0.72
(1,614)	1:38:A:LYS:HA	1:38:A:LYS:HG2	19	0.72
(1,607)	1:36:A:THR:H	1:36:A:THR:HG23	11	0.72
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	2	0.72
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	6	0.72
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG22	15	0.72
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	10	0.72
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	4	0.72
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	16	0.72
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG12	17	0.72
(1,446)	1:74:A:TYR:HA	1:74:A:TYR:HD1	7	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	17	0.72
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	20	0.72
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	20	0.72
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	8	0.72
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	18	0.72
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	9	0.72
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	13	0.72
(1,378)	1:22:A:ARG:HA	1:24:A:LEU:H	5	0.72
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	2	0.72
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	3	0.72
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	6	0.72
(1,256)	1:14:A:ARG:HD2	1:14:A:ARG:H	6	0.72
(1,256)	1:14:A:ARG:HD2	1:14:A:ARG:H	12	0.72
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	11	0.72
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	4	0.72
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	11	0.72
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	15	0.72
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	8	0.72
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	5	0.72
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	7	0.72
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	19	0.72
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	13	0.72
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	17	0.72
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	3	0.72
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	5	0.72
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	15	0.72
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	17	0.72
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	18	0.72
(1,63)	1:73:A:TYR:HD1	1:81:A:LYS:HG2	15	0.72
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	12	0.72
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	1	0.72
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	14	0.72
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	20	0.72
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	6	0.72
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	4	0.72
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	14	0.71
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	14	0.71
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	13	0.71
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	19	0.71
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	1	0.71
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	8	0.71
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	17	0.71
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	15	0.71
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	1	0.71
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	5	0.71
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	3	0.71
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	14	0.71
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	3	0.71
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	5	0.71
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	16	0.71
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	10	0.71
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	7	0.71
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	1	0.71
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	5	0.71
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	18	0.71
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD11	3	0.71
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD12	3	0.71
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD12	20	0.71
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	3	0.71
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	9	0.71
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	12	0.71
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	17	0.71
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	2	0.71
(1,1230)	1:77:A:GLN:HG3	1:77:A:GLN:HA	5	0.71
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	3	0.71
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	11	0.71
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	15	0.71
(1,1166)	1:71:A:TYR:HA	1:71:A:TYR:HD1	20	0.71
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	2	0.71
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	9	0.71
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	11	0.71
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	4	0.71
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	6	0.71
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	11	0.71
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	6	0.71
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	8	0.71
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	4	0.71
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	16	0.71
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	18	0.71
(1,953)	1:59:A:VAL:HG13	1:60:A:TYR:HD1	11	0.71
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	3	0.71
(1,865)	1:55:A:THR:HG21	1:56:A:CYS:HB3	18	0.71
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	13	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,853)	1:55:A:THR:HA	1:56:A:CYS:HB3	17	0.71
(1,828)	1:51:A:LEU:HD13	1:52:A:ASN:H	5	0.71
(1,827)	1:51:A:LEU:HD12	1:51:A:LEU:H	16	0.71
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	5	0.71
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	19	0.71
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	18	0.71
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	10	0.71
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	13	0.71
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	18	0.71
(1,752)	1:47:A:PRO:HD2	1:47:A:PRO:HB2	3	0.71
(1,752)	1:47:A:PRO:HD2	1:47:A:PRO:HB2	8	0.71
(1,752)	1:47:A:PRO:HD2	1:47:A:PRO:HB2	9	0.71
(1,752)	1:47:A:PRO:HD2	1:47:A:PRO:HB2	18	0.71
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	19	0.71
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	19	0.71
(1,722)	1:45:A:CYS:HB3	1:58:A:TYR:HE1	20	0.71
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	4	0.71
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB3	5	0.71
(1,698)	1:44:A:ALA:HB2	1:65:A:TYR:HB2	1	0.71
(1,698)	1:44:A:ALA:HB2	1:65:A:TYR:HB2	3	0.71
(1,698)	1:44:A:ALA:HB1	1:65:A:TYR:HB2	4	0.71
(1,695)	1:44:A:ALA:HB2	1:45:A:CYS:HB3	4	0.71
(1,695)	1:44:A:ALA:HB2	1:45:A:CYS:HB3	6	0.71
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	16	0.71
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	13	0.71
(1,648)	1:39:A:ASN:HB2	1:41:A:GLN:HB2	18	0.71
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	16	0.71
(1,623)	1:38:A:LYS:HB3	1:38:A:LYS:HE2	19	0.71
(1,607)	1:36:A:THR:H	1:36:A:THR:HG22	4	0.71
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG21	8	0.71
(1,599)	1:36:A:THR:HG22	1:64:A:TYR:HB3	8	0.71
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	14	0.71
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG21	10	0.71
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG23	12	0.71
(1,559)	1:33:A:LYS:HG2	1:34:A:GLY:HA3	8	0.71
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	1	0.71
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	13	0.71
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	13	0.71
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	19	0.71
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG12	6	0.71
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	1	0.71
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	2	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	5	0.71
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	11	0.71
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	15	0.71
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	4	0.71
(1,302)	1:18:A:THR:HG21	1:20:A:LYS:HD2	4	0.71
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	2	0.71
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	3	0.71
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	17	0.71
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	6	0.71
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	18	0.71
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	14	0.71
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	2	0.71
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	2	0.71
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	18	0.71
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	9	0.71
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	20	0.71
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	18	0.71
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	2	0.71
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	16	0.71
(1,19)	1:62:A:TYR:HA	1:63:A:PRO:HG2	8	0.71
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE2	1	0.71
(1,1860)	1:83:A:TYR:H	1:74:A:TYR:HD1	7	0.7
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	16	0.7
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	15	0.7
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	4	0.7
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	6	0.7
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	3	0.7
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	11	0.7
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	9	0.7
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	3	0.7
(1,1500)	1:51:A:LEU:HD22	1:50:A:CYS:H	2	0.7
(1,1481)	1:15:A:ASN:HA	1:14:A:ARG:HB2	17	0.7
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	1	0.7
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	15	0.7
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	19	0.7
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	4	0.7
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	18	0.7
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	4	0.7
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD23	13	0.7
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD11	4	0.7
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	10	0.7
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	3	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	15	0.7
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	4	0.7
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	7	0.7
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	9	0.7
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	2	0.7
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	11	0.7
(1,978)	1:60:A:TYR:H	1:60:A:TYR:HB2	14	0.7
(1,978)	1:60:A:TYR:H	1:60:A:TYR:HB2	16	0.7
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	7	0.7
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	13	0.7
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG11	10	0.7
(1,940)	1:59:A:VAL:HG11	1:66:A:LYS:HG2	13	0.7
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	1	0.7
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	17	0.7
(1,865)	1:55:A:THR:HG21	1:56:A:CYS:HB3	7	0.7
(1,865)	1:55:A:THR:HG23	1:56:A:CYS:HB3	10	0.7
(1,839)	1:53:A:GLY:HA3	1:70:A:PRO:HG3	12	0.7
(1,827)	1:51:A:LEU:HD13	1:51:A:LEU:H	8	0.7
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	3	0.7
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	4	0.7
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	20	0.7
(1,752)	1:47:A:PRO:HD2	1:47:A:PRO:HB2	19	0.7
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	15	0.7
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	2	0.7
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	7	0.7
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	9	0.7
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB1	4	0.7
(1,695)	1:44:A:ALA:HB3	1:45:A:CYS:HB3	1	0.7
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	10	0.7
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	2	0.7
(1,607)	1:36:A:THR:H	1:36:A:THR:HG23	2	0.7
(1,607)	1:36:A:THR:H	1:36:A:THR:HG21	8	0.7
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	16	0.7
(1,560)	1:34:A:GLY:HA2	1:33:A:LYS:HG2	12	0.7
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	1	0.7
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	5	0.7
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG21	2	0.7
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG13	7	0.7
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG21	5	0.7
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	16	0.7
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	2	0.7
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	11	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	17	0.7
(1,401)	1:23:A:GLY:HA3	1:24:A:LEU:HD23	4	0.7
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	9	0.7
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	16	0.7
(1,310)	1:18:A:THR:H	1:18:A:THR:HG21	10	0.7
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	4	0.7
(1,261)	1:15:A:ASN:HB3	1:16:A:GLY:HA2	15	0.7
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	12	0.7
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	7	0.7
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	14	0.7
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	5	0.7
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	10	0.7
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	15	0.7
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	18	0.7
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	8	0.7
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	14	0.7
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	16	0.7
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	3	0.7
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	2	0.7
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG23	13	0.7
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	17	0.7
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	19	0.7
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	13	0.7
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	20	0.7
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	14	0.7
(1,24)	1:78:A:CYS:HB3	1:70:A:PRO:HD3	6	0.7
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	12	0.7
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	11	0.7
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	13	0.7
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	19	0.69
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	6	0.69
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	12	0.69
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	2	0.69
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	10	0.69
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	10	0.69
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	7	0.69
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	11	0.69
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	16	0.69
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	10	0.69
(1,1634)	1:34:A:GLY:H	1:33:A:LYS:HG2	11	0.69
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	11	0.69
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	13	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	17	0.69
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	4	0.69
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	1	0.69
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	3	0.69
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	10	0.69
(1,1500)	1:51:A:LEU:HD23	1:50:A:CYS:H	20	0.69
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	2	0.69
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	4	0.69
(1,1402)	1:80:A:LEU:HD23	1:75:A:GLY:HA3	13	0.69
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	2	0.69
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	8	0.69
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	11	0.69
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	14	0.69
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	4	0.69
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	9	0.69
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	19	0.69
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	6	0.69
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	12	0.69
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	8	0.69
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	9	0.69
(1,1272)	1:79:A:GLN:HB2	1:80:A:LEU:HD22	15	0.69
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	9	0.69
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	20	0.69
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	3	0.69
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	13	0.69
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	7	0.69
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	15	0.69
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	6	0.69
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	3	0.69
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	3	0.69
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	4	0.69
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	6	0.69
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	8	0.69
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	15	0.69
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	1	0.69
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	6	0.69
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG11	10	0.69
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	5	0.69
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	2	0.69
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	10	0.69
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	18	0.69
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	7	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	15	0.69
(1,872)	1:55:A:THR:HG23	1:67:A:CYS:HA	9	0.69
(1,865)	1:55:A:THR:HG23	1:56:A:CYS:HB3	9	0.69
(1,841)	1:53:A:GLY:HA3	1:70:A:PRO:HG2	12	0.69
(1,828)	1:51:A:LEU:HD13	1:52:A:ASN:H	8	0.69
(1,828)	1:51:A:LEU:HD12	1:52:A:ASN:H	9	0.69
(1,828)	1:51:A:LEU:HD12	1:52:A:ASN:H	17	0.69
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	12	0.69
(1,787)	1:49:A:PRO:HD3	1:48:A:ASN:HB3	9	0.69
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	6	0.69
(1,752)	1:47:A:PRO:HD2	1:47:A:PRO:HB2	1	0.69
(1,752)	1:47:A:PRO:HD2	1:47:A:PRO:HB2	11	0.69
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	1	0.69
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	1	0.69
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	10	0.69
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	8	0.69
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB3	7	0.69
(1,688)	1:44:A:ALA:HA	1:36:A:THR:HG22	16	0.69
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	3	0.69
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG22	16	0.69
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	13	0.69
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	5	0.69
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	20	0.69
(1,532)	1:32:A:ARG:HD2	1:32:A:ARG:H	9	0.69
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	1	0.69
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	4	0.69
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	15	0.69
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG13	19	0.69
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	3	0.69
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	19	0.69
(1,437)	1:25:A:TYR:HB2	1:26:A:SER:HB2	3	0.69
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	1	0.69
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	12	0.69
(1,355)	1:21:A:LYS:HA	1:7:A:PRO:HG3	20	0.69
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	15	0.69
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	17	0.69
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	8	0.69
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	2	0.69
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	1	0.69
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	2	0.69
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	8	0.69
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	14	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	16	0.69
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	17	0.69
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	3	0.69
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	2	0.69
(1,84)	1:3:A:TYR:H	1:2:A:VAL:HG22	8	0.69
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	12	0.69
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	4	0.69
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	9	0.69
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	1	0.69
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	2	0.69
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	15	0.69
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	17	0.69
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	13	0.69
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	7	0.69
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	9	0.69
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	11	0.69
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	10	0.69
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	16	0.68
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	17	0.68
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	2	0.68
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	20	0.68
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	1	0.68
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	4	0.68
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	8	0.68
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	13	0.68
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	16	0.68
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	8	0.68
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	15	0.68
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	16	0.68
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	18	0.68
(1,1478)	1:18:A:THR:HG21	1:20:A:LYS:HB3	1	0.68
(1,1478)	1:18:A:THR:HG21	1:20:A:LYS:HB3	5	0.68
(1,1478)	1:18:A:THR:HG22	1:20:A:LYS:HB3	8	0.68
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	1	0.68
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	20	0.68
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	16	0.68
(1,1402)	1:80:A:LEU:HD23	1:75:A:GLY:HA3	20	0.68
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	15	0.68
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	16	0.68
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	8	0.68
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	10	0.68
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	12	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD11	13	0.68
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	1	0.68
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	19	0.68
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	1	0.68
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	11	0.68
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	12	0.68
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	18	0.68
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	8	0.68
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG21	15	0.68
(1,1054)	1:65:A:TYR:HB2	1:58:A:TYR:HD1	6	0.68
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	14	0.68
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	12	0.68
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	19	0.68
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG11	1	0.68
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	4	0.68
(1,828)	1:51:A:LEU:HD11	1:52:A:ASN:H	11	0.68
(1,827)	1:51:A:LEU:HD11	1:51:A:LEU:H	4	0.68
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	13	0.68
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	14	0.68
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	9	0.68
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	12	0.68
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	20	0.68
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	17	0.68
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	16	0.68
(1,698)	1:44:A:ALA:HB2	1:65:A:TYR:HB2	8	0.68
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	16	0.68
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	20	0.68
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG22	8	0.68
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	7	0.68
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	8	0.68
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	9	0.68
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	12	0.68
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	5	0.68
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	4	0.68
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	13	0.68
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	10	0.68
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	19	0.68
(1,307)	1:18:A:THR:HG23	1:30:A:TYR:HE1	13	0.68
(1,302)	1:18:A:THR:HG21	1:20:A:LYS:HD2	1	0.68
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	9	0.68
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	12	0.68
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	15	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	16	0.68
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	12	0.68
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	17	0.68
(1,175)	1:8:A:CYS:H	1:7:A:PRO:HD2	5	0.68
(1,175)	1:8:A:CYS:H	1:7:A:PRO:HD2	11	0.68
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	14	0.68
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	10	0.68
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	7	0.68
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	15	0.68
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	7	0.68
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG23	13	0.68
(1,104)	1:4:A:TYR:H	1:4:A:TYR:HB2	12	0.68
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	20	0.68
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	7	0.68
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	10	0.68
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	19	0.68
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	5	0.68
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	7	0.68
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	9	0.68
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	14	0.68
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	16	0.68
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	19	0.68
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	9	0.68
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	1	0.67
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	2	0.67
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	1	0.67
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	4	0.67
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	13	0.67
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	14	0.67
(1,1776)	1:65:A:TYR:H	1:59:A:VAL:HB	14	0.67
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	14	0.67
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	6	0.67
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	15	0.67
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	20	0.67
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	7	0.67
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	12	0.67
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	15	0.67
(1,1478)	1:18:A:THR:HG23	1:20:A:LYS:HB3	17	0.67
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	20	0.67
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	6	0.67
(1,1436)	1:44:A:ALA:HB2	1:58:A:TYR:HE1	4	0.67
(1,1436)	1:44:A:ALA:HB2	1:58:A:TYR:HE1	15	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	4	0.67
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	18	0.67
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	10	0.67
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	7	0.67
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD12	14	0.67
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD12	16	0.67
(1,1256)	1:78:A:CYS:HB3	1:77:A:GLN:HG3	6	0.67
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	6	0.67
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	7	0.67
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	14	0.67
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	4	0.67
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	16	0.67
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	14	0.67
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	17	0.67
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	9	0.67
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	8	0.67
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	20	0.67
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	10	0.67
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	12	0.67
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	8	0.67
(1,976)	1:60:A:TYR:HB2	1:60:A:TYR:HD1	14	0.67
(1,973)	1:74:A:TYR:HB2	1:82:A:LYS:HB3	15	0.67
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	12	0.67
(1,828)	1:51:A:LEU:HD13	1:52:A:ASN:H	10	0.67
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	20	0.67
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	2	0.67
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	3	0.67
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	5	0.67
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	8	0.67
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	15	0.67
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	13	0.67
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	19	0.67
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB2	1	0.67
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB1	15	0.67
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB2	18	0.67
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG21	9	0.67
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	11	0.67
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	13	0.67
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG23	19	0.67
(1,560)	1:34:A:GLY:HA2	1:33:A:LYS:HG2	8	0.67
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	5	0.67
(1,552)	1:33:A:LYS:HB2	1:33:A:LYS:H	20	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	20	0.67
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	9	0.67
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	13	0.67
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	16	0.67
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	10	0.67
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	1	0.67
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	17	0.67
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	4	0.67
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	1	0.67
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	7	0.67
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG22	7	0.67
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG22	8	0.67
(1,310)	1:18:A:THR:H	1:18:A:THR:HG23	12	0.67
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	3	0.67
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	18	0.67
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	3	0.67
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	11	0.67
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	13	0.67
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	1	0.67
(1,153)	1:83:A:TYR:H	1:83:A:TYR:HB3	17	0.67
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	3	0.67
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	7	0.67
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	3	0.67
(1,122)	1:5:A:PRO:HB3	1:3:A:TYR:HE1	19	0.67
(1,84)	1:3:A:TYR:H	1:2:A:VAL:HG23	4	0.67
(1,83)	1:2:A:VAL:HG23	1:4:A:TYR:HE1	8	0.67
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	14	0.67
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	8	0.67
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	10	0.67
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	13	0.67
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	18	0.67
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	20	0.67
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	4	0.67
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	11	0.67
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	19	0.67
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	12	0.67
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	7	0.66
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	20	0.66
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	15	0.66
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	3	0.66
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	15	0.66
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	10	0.66
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	11	0.66
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	1	0.66
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	15	0.66
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	11	0.66
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	11	0.66
(1,1436)	1:44:A:ALA:HB3	1:58:A:TYR:HE1	1	0.66
(1,1402)	1:80:A:LEU:HD22	1:75:A:GLY:HA3	15	0.66
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	1	0.66
(1,1390)	1:83:A:TYR:HA	1:83:A:TYR:HD1	15	0.66
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	9	0.66
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	7	0.66
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	16	0.66
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	8	0.66
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	15	0.66
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	12	0.66
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	19	0.66
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	12	0.66
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	10	0.66
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	14	0.66
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	7	0.66
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	1	0.66
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	5	0.66
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	3	0.66
(1,953)	1:59:A:VAL:HG13	1:60:A:TYR:HD1	2	0.66
(1,940)	1:59:A:VAL:HG13	1:66:A:LYS:HG2	10	0.66
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	7	0.66
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	3	0.66
(1,828)	1:51:A:LEU:HD13	1:52:A:ASN:H	1	0.66
(1,828)	1:51:A:LEU:HD13	1:52:A:ASN:H	14	0.66
(1,827)	1:51:A:LEU:HD12	1:51:A:LEU:H	13	0.66
(1,787)	1:49:A:PRO:HD3	1:48:A:ASN:HB3	7	0.66
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	7	0.66
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	16	0.66
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	18	0.66
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	4	0.66
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	5	0.66
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	20	0.66
(1,706)	1:44:A:ALA:HB1	1:64:A:TYR:HD1	10	0.66
(1,701)	1:43:A:ASN:HA	1:44:A:ALA:HB2	2	0.66
(1,695)	1:44:A:ALA:HB3	1:45:A:CYS:HB3	8	0.66
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG21	19	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG21	20	0.66
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	13	0.66
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	16	0.66
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	10	0.66
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	13	0.66
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	7	0.66
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	4	0.66
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	14	0.66
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	19	0.66
(1,488)	1:28:A:LYS:HE2	1:28:A:LYS:HA	17	0.66
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	6	0.66
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG11	11	0.66
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	11	0.66
(1,439)	1:25:A:TYR:HB2	1:25:A:TYR:HD1	15	0.66
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	9	0.66
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	20	0.66
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	6	0.66
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	11	0.66
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	19	0.66
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	9	0.66
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	11	0.66
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	8	0.66
(1,389)	1:22:A:ARG:HG3	1:21:A:LYS:HA	14	0.66
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	20	0.66
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG21	5	0.66
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	19	0.66
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	10	0.66
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	19	0.66
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	12	0.66
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	17	0.66
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	18	0.66
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	2	0.66
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	11	0.66
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	19	0.66
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	15	0.66
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	11	0.66
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	15	0.66
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG21	7	0.66
(1,70)	1:30:A:TYR:HE1	1:30:A:TYR:HB3	1	0.66
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	3	0.66
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	4	0.66
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	8	0.66
(1,27)	1:28:A:LYS:H	1:28:A:LYS:HD2	17	0.66
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	1	0.66
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	20	0.66
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	4	0.66
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	1	0.65
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	12	0.65
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	18	0.65
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	6	0.65
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	3	0.65
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	17	0.65
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	15	0.65
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	17	0.65
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	13	0.65
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	12	0.65
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	17	0.65
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	18	0.65
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	1	0.65
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	14	0.65
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	19	0.65
(1,1478)	1:18:A:THR:HG21	1:20:A:LYS:HB3	10	0.65
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	13	0.65
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	9	0.65
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	8	0.65
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	1	0.65
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	2	0.65
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	3	0.65
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	4	0.65
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	5	0.65
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	6	0.65
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	7	0.65
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	8	0.65
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	11	0.65
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	12	0.65
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	17	0.65
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	20	0.65
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD23	18	0.65
(1,1291)	1:80:A:LEU:HA	1:81:A:LYS:HB3	10	0.65
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	6	0.65
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	19	0.65
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	8	0.65
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	11	0.65
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	18	0.65
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	4	0.65
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	13	0.65
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	10	0.65
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	13	0.65
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	6	0.65
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	1	0.65
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	12	0.65
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	13	0.65
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	18	0.65
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	3	0.65
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	12	0.65
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	16	0.65
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	15	0.65
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG12	19	0.65
(1,948)	1:59:A:VAL:HG11	1:64:A:TYR:HA	9	0.65
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	14	0.65
(1,872)	1:55:A:THR:HG21	1:67:A:CYS:HA	19	0.65
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	19	0.65
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	7	0.65
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	13	0.65
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	10	0.65
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	11	0.65
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	13	0.65
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	15	0.65
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	17	0.65
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	5	0.65
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	16	0.65
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	16	0.65
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	1	0.65
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	14	0.65
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	11	0.65
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG21	5	0.65
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG23	2	0.65
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG23	12	0.65
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG21	18	0.65
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	2	0.65
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG13	12	0.65
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG13	13	0.65
(1,453)	1:22:A:ARG:HG2	1:27:A:TYR:HA	3	0.65
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	19	0.65
(1,412)	1:24:A:LEU:H	1:24:A:LEU:HD22	3	0.65
(1,412)	1:24:A:LEU:H	1:24:A:LEU:HD23	7	0.65
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	9	0.65
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	2	0.65
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	14	0.65
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	16	0.65
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	16	0.65
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	20	0.65
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	14	0.65
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG22	18	0.65
(1,310)	1:18:A:THR:H	1:18:A:THR:HG22	3	0.65
(1,310)	1:18:A:THR:H	1:18:A:THR:HG21	5	0.65
(1,302)	1:18:A:THR:HG23	1:20:A:LYS:HD2	17	0.65
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	16	0.65
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	6	0.65
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	9	0.65
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	6	0.65
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	13	0.65
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	19	0.65
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	7	0.65
(1,214)	1:10:A:PRO:HB3	1:10:A:PRO:HD2	20	0.65
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	12	0.65
(1,191)	1:8:A:CYS:HB3	1:9:A:SER:HB2	13	0.65
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	5	0.65
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	14	0.65
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	18	0.65
(1,103)	1:4:A:TYR:HB2	1:4:A:TYR:HD1	12	0.65
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG23	16	0.65
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	11	0.65
(1,64)	1:73:A:TYR:HE1	1:73:A:TYR:HB3	12	0.65
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	5	0.65
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	3	0.64
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	6	0.64
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	8	0.64
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	9	0.64
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	10	0.64
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	15	0.64
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	20	0.64
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	10	0.64
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	1	0.64
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	4	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	10	0.64
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	16	0.64
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	19	0.64
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	3	0.64
(1,1671)	1:41:A:GLN:H	1:39:A:ASN:HB3	16	0.64
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	17	0.64
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	9	0.64
(1,1539)	1:17:A:GLY:H	1:32:A:ARG:HG2	17	0.64
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	6	0.64
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	5	0.64
(1,1478)	1:18:A:THR:HG22	1:20:A:LYS:HB3	2	0.64
(1,1467)	1:22:A:ARG:HD2	1:22:A:ARG:H	6	0.64
(1,1459)	1:14:A:ARG:HG2	1:14:A:ARG:HD2	1	0.64
(1,1459)	1:14:A:ARG:HG2	1:14:A:ARG:HD2	3	0.64
(1,1459)	1:14:A:ARG:HG2	1:14:A:ARG:HD2	6	0.64
(1,1451)	1:33:A:LYS:HB2	1:32:A:ARG:HA	12	0.64
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	6	0.64
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	13	0.64
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	16	0.64
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	2	0.64
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	19	0.64
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	4	0.64
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	13	0.64
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	6	0.64
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	11	0.64
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD13	12	0.64
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	17	0.64
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	1	0.64
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	7	0.64
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	10	0.64
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	1	0.64
(1,1166)	1:71:A:TYR:HA	1:71:A:TYR:HD1	9	0.64
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	4	0.64
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	6	0.64
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	5	0.64
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	4	0.64
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	5	0.64
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	5	0.64
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	14	0.64
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	13	0.64
(1,1036)	1:59:A:VAL:HG11	1:65:A:TYR:HA	11	0.64
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	17	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	8	0.64
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	8	0.64
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	17	0.64
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG11	10	0.64
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	20	0.64
(1,872)	1:55:A:THR:HG22	1:67:A:CYS:HA	3	0.64
(1,872)	1:55:A:THR:HG21	1:67:A:CYS:HA	4	0.64
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	5	0.64
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	9	0.64
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	4	0.64
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	6	0.64
(1,745)	1:47:A:PRO:HB2	1:47:A:PRO:HD3	14	0.64
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	2	0.64
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	10	0.64
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	12	0.64
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	18	0.64
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	5	0.64
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	6	0.64
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB2	8	0.64
(1,698)	1:44:A:ALA:HB3	1:65:A:TYR:HB2	14	0.64
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	20	0.64
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG23	6	0.64
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG22	10	0.64
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	8	0.64
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	2	0.64
(1,564)	1:34:A:GLY:HA3	1:58:A:TYR:HE1	7	0.64
(1,564)	1:34:A:GLY:HA3	1:58:A:TYR:HE1	13	0.64
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	10	0.64
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	16	0.64
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	6	0.64
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	7	0.64
(1,488)	1:28:A:LYS:HE2	1:28:A:LYS:HA	4	0.64
(1,478)	1:66:A:LYS:HB2	1:66:A:LYS:HE2	8	0.64
(1,469)	1:66:A:LYS:HA	1:66:A:LYS:HG2	6	0.64
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	4	0.64
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	5	0.64
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	7	0.64
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	8	0.64
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	12	0.64
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	10	0.64
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	15	0.64
(1,332)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	14	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	5	0.64
(1,310)	1:18:A:THR:H	1:18:A:THR:HG22	11	0.64
(1,310)	1:18:A:THR:H	1:18:A:THR:HG23	15	0.64
(1,310)	1:18:A:THR:H	1:18:A:THR:HG21	19	0.64
(1,302)	1:18:A:THR:HG22	1:20:A:LYS:HD2	8	0.64
(1,302)	1:18:A:THR:HG21	1:20:A:LYS:HD2	10	0.64
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	16	0.64
(1,235)	1:11:A:TYR:HA	1:11:A:TYR:HD1	11	0.64
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	17	0.64
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	10	0.64
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	11	0.64
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	19	0.64
(1,175)	1:8:A:CYS:H	1:7:A:PRO:HD2	10	0.64
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	7	0.64
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	8	0.64
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	14	0.64
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	18	0.64
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	11	0.64
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	14	0.64
(1,84)	1:3:A:TYR:H	1:2:A:VAL:HG21	1	0.64
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	1	0.64
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	19	0.64
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	14	0.64
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	13	0.63
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	2	0.63
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	5	0.63
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	7	0.63
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	9	0.63
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	5	0.63
(1,1745)	1:57:A:GLY:H	1:65:A:TYR:HD1	1	0.63
(1,1698)	1:44:A:ALA:H	1:58:A:TYR:HE1	13	0.63
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	11	0.63
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	20	0.63
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	1	0.63
(1,1540)	1:17:A:GLY:H	1:13:A:CYS:HB2	20	0.63
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	18	0.63
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	11	0.63
(1,1459)	1:14:A:ARG:HG2	1:14:A:ARG:HD2	2	0.63
(1,1459)	1:14:A:ARG:HG2	1:14:A:ARG:HD2	5	0.63
(1,1459)	1:14:A:ARG:HG2	1:14:A:ARG:HD2	12	0.63
(1,1459)	1:14:A:ARG:HG2	1:14:A:ARG:HD2	19	0.63
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	10	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	8	0.63
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	5	0.63
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	20	0.63
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	20	0.63
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	4	0.63
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	4	0.63
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	3	0.63
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	4	0.63
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	7	0.63
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	17	0.63
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	8	0.63
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	5	0.63
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	14	0.63
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	17	0.63
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	19	0.63
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	18	0.63
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	12	0.63
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	13	0.63
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	15	0.63
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	9	0.63
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	13	0.63
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	7	0.63
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	4	0.63
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	14	0.63
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	16	0.63
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	18	0.63
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	4	0.63
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	20	0.63
(1,977)	1:60:A:TYR:HB3	1:60:A:TYR:HD1	5	0.63
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	13	0.63
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	12	0.63
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	1	0.63
(1,828)	1:51:A:LEU:HD12	1:52:A:ASN:H	16	0.63
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	11	0.63
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	14	0.63
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	3	0.63
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	5	0.63
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	6	0.63
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	3	0.63
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	4	0.63
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	14	0.63
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	2	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,617)	1:38:A:LYS:HA	1:38:A:LYS:HE3	20	0.63
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG21	18	0.63
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	12	0.63
(1,553)	1:33:A:LYS:HB3	1:33:A:LYS:H	11	0.63
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	15	0.63
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	2	0.63
(1,527)	1:32:A:ARG:HD2	1:32:A:ARG:HG2	4	0.63
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	8	0.63
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG22	9	0.63
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	16	0.63
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	1	0.63
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	3	0.63
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	4	0.63
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	5	0.63
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	13	0.63
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	20	0.63
(1,347)	1:20:A:LYS:HG2	1:20:A:LYS:HE2	3	0.63
(1,347)	1:20:A:LYS:HG2	1:20:A:LYS:HE2	9	0.63
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	2	0.63
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	6	0.63
(1,310)	1:18:A:THR:H	1:18:A:THR:HG22	7	0.63
(1,310)	1:18:A:THR:H	1:18:A:THR:HG23	20	0.63
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	3	0.63
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	8	0.63
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	10	0.63
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	4	0.63
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	9	0.63
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	10	0.63
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	19	0.63
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	15	0.63
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	7	0.63
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	11	0.63
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG22	6	0.63
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	19	0.63
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	3	0.63
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	11	0.63
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	15	0.63
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	10	0.63
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	5	0.63
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	20	0.63
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	3	0.63
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	1	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	12	0.62
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	7	0.62
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	3	0.62
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	19	0.62
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	10	0.62
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	2	0.62
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	2	0.62
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	17	0.62
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	10	0.62
(1,1603)	1:29:A:CYS:H	1:28:A:LYS:HE3	12	0.62
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	2	0.62
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	10	0.62
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	19	0.62
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	18	0.62
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	12	0.62
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	9	0.62
(1,1454)	1:33:A:LYS:HG2	1:33:A:LYS:HE3	20	0.62
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	15	0.62
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	19	0.62
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	3	0.62
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	9	0.62
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	9	0.62
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	3	0.62
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD22	11	0.62
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD23	17	0.62
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD11	11	0.62
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	20	0.62
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	2	0.62
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	13	0.62
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	20	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	1	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	2	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	3	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	4	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	5	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	6	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	7	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	8	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	9	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	10	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	11	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	12	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	13	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	14	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	15	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	16	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	17	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	18	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	19	0.62
(1,1222)	1:76:A:LYS:HA	1:76:A:LYS:HB2	20	0.62
(1,1191)	1:73:A:TYR:HB3	1:70:A:PRO:HD3	12	0.62
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	6	0.62
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	7	0.62
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	9	0.62
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	16	0.62
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	18	0.62
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	5	0.62
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	16	0.62
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	4	0.62
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	4	0.62
(1,1101)	1:69:A:CYS:HB2	1:78:A:CYS:HB2	11	0.62
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	20	0.62
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	9	0.62
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	19	0.62
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	9	0.62
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	18	0.62
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG12	19	0.62
(1,940)	1:59:A:VAL:HG13	1:66:A:LYS:HG2	17	0.62
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	16	0.62
(1,872)	1:55:A:THR:HG23	1:67:A:CYS:HA	10	0.62
(1,865)	1:55:A:THR:HG21	1:56:A:CYS:HB3	4	0.62
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	4	0.62
(1,828)	1:51:A:LEU:HD11	1:52:A:ASN:H	4	0.62
(1,824)	1:51:A:LEU:HD23	1:51:A:LEU:H	20	0.62
(1,822)	1:51:A:LEU:HD21	1:56:A:CYS:HB3	20	0.62
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	9	0.62
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	12	0.62
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	4	0.62
(1,763)	1:48:A:ASN:HA	1:47:A:PRO:HB3	15	0.62
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	4	0.62
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	2	0.62
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	3	0.62
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	2	0.62
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	15	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB1	11	0.62
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	3	0.62
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	4	0.62
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	9	0.62
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	7	0.62
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	17	0.62
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	18	0.62
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	14	0.62
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	16	0.62
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	7	0.62
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	15	0.62
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	15	0.62
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	8	0.62
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	14	0.62
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	12	0.62
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	10	0.62
(1,527)	1:32:A:ARG:HD2	1:32:A:ARG:HG2	2	0.62
(1,527)	1:32:A:ARG:HD2	1:32:A:ARG:HG2	12	0.62
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	17	0.62
(1,470)	1:66:A:LYS:HA	1:67:A:CYS:HB2	10	0.62
(1,412)	1:24:A:LEU:H	1:24:A:LEU:HD21	11	0.62
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	7	0.62
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	16	0.62
(1,347)	1:20:A:LYS:HG2	1:20:A:LYS:HE2	11	0.62
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG21	1	0.62
(1,310)	1:18:A:THR:H	1:18:A:THR:HG22	2	0.62
(1,310)	1:18:A:THR:H	1:18:A:THR:HG22	14	0.62
(1,310)	1:18:A:THR:H	1:18:A:THR:HG23	17	0.62
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	19	0.62
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	12	0.62
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	18	0.62
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	10	0.62
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	6	0.62
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	2	0.62
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	8	0.62
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	13	0.62
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	6	0.62
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	13	0.62
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	6	0.62
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	12	0.62
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	4	0.62
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	10	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	7	0.62
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	17	0.62
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	11	0.62
(1,61)	1:71:A:TYR:HE1	1:71:A:TYR:HA	10	0.62
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	17	0.62
(1,1858)	1:83:A:TYR:H	1:82:A:LYS:HB2	20	0.61
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	5	0.61
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	20	0.61
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	18	0.61
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	8	0.61
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	11	0.61
(1,1740)	1:57:A:GLY:H	1:66:A:LYS:HB2	1	0.61
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	15	0.61
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD13	4	0.61
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	4	0.61
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	11	0.61
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	14	0.61
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	13	0.61
(1,1518)	1:8:A:CYS:H	1:9:A:SER:HB2	11	0.61
(1,1469)	1:22:A:ARG:HB3	1:22:A:ARG:HD2	6	0.61
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	4	0.61
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	6	0.61
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	12	0.61
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	13	0.61
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	16	0.61
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	19	0.61
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	14	0.61
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	8	0.61
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	16	0.61
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	18	0.61
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	3	0.61
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	4	0.61
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	17	0.61
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD23	1	0.61
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	11	0.61
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	13	0.61
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	14	0.61
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	16	0.61
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	7	0.61
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD12	1	0.61
(1,1182)	1:72:A:GLY:HA2	1:71:A:TYR:HD1	18	0.61
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	4	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	17	0.61
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	1	0.61
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	2	0.61
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	10	0.61
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	11	0.61
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	13	0.61
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	15	0.61
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	20	0.61
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	17	0.61
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	20	0.61
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	5	0.61
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	2	0.61
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	9	0.61
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	11	0.61
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	7	0.61
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	8	0.61
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	8	0.61
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	16	0.61
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	2	0.61
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	13	0.61
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	4	0.61
(1,1063)	1:66:A:LYS:HG2	1:59:A:VAL:HG21	3	0.61
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	6	0.61
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	13	0.61
(1,976)	1:60:A:TYR:HB2	1:60:A:TYR:HD1	16	0.61
(1,943)	1:59:A:VAL:HG11	1:65:A:TYR:HB3	9	0.61
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	9	0.61
(1,872)	1:55:A:THR:HG23	1:67:A:CYS:HA	2	0.61
(1,872)	1:55:A:THR:HG22	1:67:A:CYS:HA	12	0.61
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	16	0.61
(1,828)	1:51:A:LEU:HD13	1:52:A:ASN:H	6	0.61
(1,822)	1:51:A:LEU:HD22	1:56:A:CYS:HB3	1	0.61
(1,822)	1:51:A:LEU:HD22	1:56:A:CYS:HB3	15	0.61
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	13	0.61
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	16	0.61
(1,762)	1:48:A:ASN:HA	1:49:A:PRO:HB3	19	0.61
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	6	0.61
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	15	0.61
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	16	0.61
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	3	0.61
(1,617)	1:38:A:LYS:HA	1:38:A:LYS:HE3	1	0.61
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG23	14	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG22	18	0.61
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG23	9	0.61
(1,600)	1:36:A:THR:HG21	1:64:A:TYR:HB2	2	0.61
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	18	0.61
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	1	0.61
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	8	0.61
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	17	0.61
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	15	0.61
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	12	0.61
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	13	0.61
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	16	0.61
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	12	0.61
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	6	0.61
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	9	0.61
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	6	0.61
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	18	0.61
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	13	0.61
(1,401)	1:23:A:GLY:HA3	1:24:A:LEU:HD21	11	0.61
(1,365)	1:21:A:LYS:HE2	1:21:A:LYS:HD3	1	0.61
(1,365)	1:21:A:LYS:HE2	1:21:A:LYS:HD3	3	0.61
(1,365)	1:21:A:LYS:HE2	1:21:A:LYS:HD3	10	0.61
(1,365)	1:21:A:LYS:HE2	1:21:A:LYS:HD3	12	0.61
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	2	0.61
(1,310)	1:18:A:THR:H	1:18:A:THR:HG23	13	0.61
(1,310)	1:18:A:THR:H	1:18:A:THR:HG22	18	0.61
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	4	0.61
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	9	0.61
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	14	0.61
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	3	0.61
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	4	0.61
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	6	0.61
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	9	0.61
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	14	0.61
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	16	0.61
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	2	0.61
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	18	0.61
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	6	0.61
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	14	0.61
(1,61)	1:71:A:TYR:HE1	1:71:A:TYR:HA	6	0.61
(1,38)	1:82:A:LYS:H	1:74:A:TYR:HE1	19	0.61
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	1	0.61
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	15	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	10	0.61
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	11	0.6
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	14	0.6
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	16	0.6
(1,1857)	1:83:A:TYR:H	1:82:A:LYS:HG2	5	0.6
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	1	0.6
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	4	0.6
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	2	0.6
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	5	0.6
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	2	0.6
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	14	0.6
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	17	0.6
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	20	0.6
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	15	0.6
(1,1620)	1:31:A:CYS:H	1:18:A:THR:HB	2	0.6
(1,1620)	1:31:A:CYS:H	1:18:A:THR:HB	18	0.6
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	16	0.6
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	7	0.6
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	3	0.6
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	15	0.6
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	5	0.6
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	2	0.6
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	1	0.6
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	3	0.6
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	5	0.6
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	9	0.6
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	14	0.6
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	18	0.6
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	13	0.6
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	7	0.6
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	19	0.6
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	2	0.6
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	9	0.6
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	12	0.6
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	20	0.6
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	12	0.6
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD13	5	0.6
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD12	3	0.6
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	6	0.6
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	4	0.6
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	3	0.6
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	8	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	7	0.6
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	7	0.6
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	9	0.6
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	10	0.6
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	10	0.6
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	2	0.6
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	13	0.6
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	1	0.6
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	11	0.6
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	2	0.6
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	11	0.6
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	2	0.6
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG13	20	0.6
(1,940)	1:59:A:VAL:HG11	1:66:A:LYS:HG2	19	0.6
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	19	0.6
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	14	0.6
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	17	0.6
(1,872)	1:55:A:THR:HG21	1:67:A:CYS:HA	6	0.6
(1,822)	1:51:A:LEU:HD22	1:56:A:CYS:HB3	8	0.6
(1,822)	1:51:A:LEU:HD22	1:56:A:CYS:HB3	16	0.6
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	4	0.6
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	11	0.6
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	7	0.6
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	4	0.6
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	6	0.6
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	7	0.6
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB1	6	0.6
(1,704)	1:44:A:ALA:HB3	1:35:A:TYR:HA	20	0.6
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	13	0.6
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	19	0.6
(1,623)	1:38:A:LYS:HB3	1:38:A:LYS:HE2	3	0.6
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG23	11	0.6
(1,579)	1:35:A:TYR:HA	1:40:A:CYS:HB2	5	0.6
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	3	0.6
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	15	0.6
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	17	0.6
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	12	0.6
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	1	0.6
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	16	0.6
(1,483)	1:28:A:LYS:HB3	1:28:A:LYS:HE2	2	0.6
(1,483)	1:28:A:LYS:HB3	1:28:A:LYS:HE2	4	0.6
(1,483)	1:28:A:LYS:HB3	1:28:A:LYS:HE2	20	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	14	0.6
(1,406)	1:24:A:LEU:H	1:23:A:GLY:HA3	7	0.6
(1,365)	1:21:A:LYS:HE2	1:21:A:LYS:HD3	2	0.6
(1,365)	1:21:A:LYS:HE2	1:21:A:LYS:HD3	9	0.6
(1,365)	1:21:A:LYS:HE2	1:21:A:LYS:HD3	15	0.6
(1,365)	1:21:A:LYS:HE2	1:21:A:LYS:HD3	17	0.6
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	11	0.6
(1,310)	1:18:A:THR:H	1:18:A:THR:HG21	9	0.6
(1,302)	1:18:A:THR:HG22	1:20:A:LYS:HD2	2	0.6
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	4	0.6
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	1	0.6
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	8	0.6
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	16	0.6
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	15	0.6
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	2	0.6
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	4	0.6
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	6	0.6
(1,175)	1:8:A:CYS:H	1:7:A:PRO:HD2	16	0.6
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	4	0.6
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	16	0.6
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	20	0.6
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	11	0.6
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	20	0.6
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	6	0.6
(1,83)	1:2:A:VAL:HG21	1:4:A:TYR:HE1	4	0.6
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	8	0.6
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	9	0.6
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	2	0.6
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	3	0.6
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	13	0.6
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	10	0.6
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	4	0.59
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	16	0.59
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	1	0.59
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	19	0.59
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	16	0.59
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	6	0.59
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	13	0.59
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	15	0.59
(1,1671)	1:41:A:GLN:H	1:39:A:ASN:HB3	6	0.59
(1,1603)	1:29:A:CYS:H	1:28:A:LYS:HE3	5	0.59
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	5	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	6	0.59
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	12	0.59
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	9	0.59
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	19	0.59
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	9	0.59
(1,1522)	1:8:A:CYS:H	1:9:A:SER:H	10	0.59
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	8	0.59
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG13	7	0.59
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG13	20	0.59
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	10	0.59
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	2	0.59
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	11	0.59
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	14	0.59
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	4	0.59
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	5	0.59
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	10	0.59
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	16	0.59
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	18	0.59
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	10	0.59
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	3	0.59
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	16	0.59
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	6	0.59
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD22	19	0.59
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	5	0.59
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	15	0.59
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	18	0.59
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	16	0.59
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	7	0.59
(1,1191)	1:73:A:TYR:HB3	1:70:A:PRO:HD3	3	0.59
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	18	0.59
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	12	0.59
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	5	0.59
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	16	0.59
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	9	0.59
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	10	0.59
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	16	0.59
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	16	0.59
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	5	0.59
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	5	0.59
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	1	0.59
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	4	0.59
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	11	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	7	0.59
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	10	0.59
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	18	0.59
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	10	0.59
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	19	0.59
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	7	0.59
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	11	0.59
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	14	0.59
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	18	0.59
(1,965)	1:59:A:VAL:HG23	1:64:A:TYR:H	20	0.59
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG11	6	0.59
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG12	7	0.59
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	4	0.59
(1,828)	1:51:A:LEU:HD13	1:52:A:ASN:H	3	0.59
(1,828)	1:51:A:LEU:HD12	1:52:A:ASN:H	7	0.59
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	18	0.59
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	8	0.59
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	17	0.59
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	15	0.59
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	19	0.59
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	15	0.59
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	10	0.59
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB2	20	0.59
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	20	0.59
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG23	16	0.59
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG23	20	0.59
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	18	0.59
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	9	0.59
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	12	0.59
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	1	0.59
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	18	0.59
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	19	0.59
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	9	0.59
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	20	0.59
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	14	0.59
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	17	0.59
(1,431)	1:25:A:TYR:HA	1:25:A:TYR:HD1	13	0.59
(1,365)	1:21:A:LYS:HE2	1:21:A:LYS:HD3	16	0.59
(1,302)	1:18:A:THR:HG22	1:20:A:LYS:HD2	7	0.59
(1,302)	1:18:A:THR:HG21	1:20:A:LYS:HD2	16	0.59
(1,302)	1:18:A:THR:HG23	1:20:A:LYS:HD2	20	0.59
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	5	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	7	0.59
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	10	0.59
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	20	0.59
(1,175)	1:8:A:CYS:H	1:7:A:PRO:HD2	4	0.59
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	5	0.59
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	6	0.59
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	19	0.59
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	12	0.59
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	1	0.59
(1,97)	1:4:A:TYR:HA	1:5:A:PRO:HG2	1	0.59
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	1	0.59
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	2	0.59
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	20	0.59
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	17	0.59
(1,61)	1:71:A:TYR:HE1	1:71:A:TYR:HA	5	0.59
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	11	0.59
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	19	0.59
(1,23)	1:78:A:CYS:HB2	1:70:A:PRO:HD3	4	0.59
(1,23)	1:78:A:CYS:HB2	1:70:A:PRO:HD3	13	0.59
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	15	0.59
(1,12)	1:34:A:GLY:HA3	1:58:A:TYR:HB3	18	0.59
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	6	0.58
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	10	0.58
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	9	0.58
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	15	0.58
(1,1838)	1:77:A:GLN:H	1:77:A:GLN:HG3	11	0.58
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	5	0.58
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	11	0.58
(1,1712)	1:48:A:ASN:H	1:48:A:ASN:HB3	10	0.58
(1,1576)	1:24:A:LEU:H	1:24:A:LEU:HB3	1	0.58
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	2	0.58
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	12	0.58
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	14	0.58
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG12	3	0.58
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG11	6	0.58
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG12	9	0.58
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG12	13	0.58
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG11	14	0.58
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG13	17	0.58
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG13	18	0.58
(1,1478)	1:18:A:THR:HG21	1:20:A:LYS:HB3	4	0.58
(1,1454)	1:33:A:LYS:HG2	1:33:A:LYS:HE3	13	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	7	0.58
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	8	0.58
(1,1449)	1:33:A:LYS:HA	1:34:A:GLY:HA3	17	0.58
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	1	0.58
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	12	0.58
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	12	0.58
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	15	0.58
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	16	0.58
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	3	0.58
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	11	0.58
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	2	0.58
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	11	0.58
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	8	0.58
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	3	0.58
(1,1315)	1:80:A:LEU:H	1:80:A:LEU:HD11	7	0.58
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	1	0.58
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	11	0.58
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	13	0.58
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	12	0.58
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	12	0.58
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD11	7	0.58
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	9	0.58
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	11	0.58
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	13	0.58
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	20	0.58
(1,1164)	1:71:A:TYR:HA	1:72:A:GLY:HA2	4	0.58
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	8	0.58
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	12	0.58
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	16	0.58
(1,1110)	1:69:A:CYS:HB2	1:75:A:GLY:H	11	0.58
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	2	0.58
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	9	0.58
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	14	0.58
(1,1039)	1:58:A:TYR:HB2	1:65:A:TYR:HA	14	0.58
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	17	0.58
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG13	1	0.58
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG12	6	0.58
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	18	0.58
(1,828)	1:51:A:LEU:HD12	1:52:A:ASN:H	13	0.58
(1,827)	1:51:A:LEU:HD12	1:51:A:LEU:H	9	0.58
(1,827)	1:51:A:LEU:HD12	1:51:A:LEU:H	15	0.58
(1,822)	1:51:A:LEU:HD23	1:56:A:CYS:HB3	13	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	6	0.58
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	20	0.58
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	9	0.58
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	9	0.58
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	13	0.58
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	20	0.58
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	18	0.58
(1,698)	1:44:A:ALA:HB3	1:65:A:TYR:HB2	2	0.58
(1,695)	1:44:A:ALA:HB1	1:45:A:CYS:HB3	5	0.58
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	15	0.58
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	19	0.58
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	20	0.58
(1,607)	1:36:A:THR:H	1:36:A:THR:HG22	1	0.58
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG22	14	0.58
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	17	0.58
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	6	0.58
(1,559)	1:33:A:LYS:HG2	1:34:A:GLY:HA3	20	0.58
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	10	0.58
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	11	0.58
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	15	0.58
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	20	0.58
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	7	0.58
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	10	0.58
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	1	0.58
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	18	0.58
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	16	0.58
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD21	6	0.58
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	14	0.58
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG22	3	0.58
(1,310)	1:18:A:THR:H	1:18:A:THR:HG22	8	0.58
(1,310)	1:18:A:THR:H	1:18:A:THR:HG21	16	0.58
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	15	0.58
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	2	0.58
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	3	0.58
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	6	0.58
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	4	0.58
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	17	0.58
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	5	0.58
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	9	0.58
(1,130)	1:5:A:PRO:HD3	1:2:A:VAL:HG22	3	0.58
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	5	0.58
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	18	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	3	0.58
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	8	0.58
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	12	0.58
(1,84)	1:3:A:TYR:H	1:2:A:VAL:HG21	2	0.58
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	10	0.58
(1,21)	1:69:A:CYS:HA	1:70:A:PRO:HG2	6	0.58
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	12	0.57
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	19	0.57
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	14	0.57
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	3	0.57
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	7	0.57
(1,1634)	1:34:A:GLY:H	1:33:A:LYS:HG2	12	0.57
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	17	0.57
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	10	0.57
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	17	0.57
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG13	5	0.57
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG12	15	0.57
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG12	16	0.57
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	2	0.57
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	15	0.57
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	15	0.57
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	3	0.57
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	6	0.57
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	17	0.57
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	5	0.57
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	10	0.57
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	12	0.57
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	4	0.57
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	8	0.57
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	10	0.57
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	11	0.57
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	5	0.57
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	18	0.57
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	13	0.57
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	1	0.57
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	2	0.57
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	3	0.57
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	20	0.57
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	15	0.57
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	2	0.57
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	1	0.57
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	1	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	20	0.57
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	14	0.57
(1,1110)	1:69:A:CYS:HB2	1:75:A:GLY:H	4	0.57
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	14	0.57
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	3	0.57
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	3	0.57
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	8	0.57
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	3	0.57
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	19	0.57
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	2	0.57
(1,976)	1:60:A:TYR:HB2	1:60:A:TYR:HD1	9	0.57
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	2	0.57
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG12	12	0.57
(1,940)	1:59:A:VAL:HG13	1:66:A:LYS:HG2	5	0.57
(1,940)	1:59:A:VAL:HG12	1:66:A:LYS:HG2	16	0.57
(1,922)	1:59:A:VAL:HA	1:66:A:LYS:HG3	3	0.57
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	3	0.57
(1,828)	1:51:A:LEU:HD11	1:52:A:ASN:H	19	0.57
(1,827)	1:51:A:LEU:HD13	1:51:A:LEU:H	5	0.57
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	12	0.57
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	13	0.57
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	16	0.57
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	1	0.57
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	7	0.57
(1,720)	1:45:A:CYS:HA	1:44:A:ALA:H	16	0.57
(1,695)	1:44:A:ALA:HB2	1:45:A:CYS:HB3	11	0.57
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	19	0.57
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	4	0.57
(1,597)	1:36:A:THR:HG21	1:42:A:TYR:HB3	3	0.57
(1,551)	1:33:A:LYS:HB3	1:33:A:LYS:HE2	6	0.57
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	3	0.57
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	7	0.57
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	9	0.57
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	13	0.57
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	2	0.57
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	16	0.57
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	8	0.57
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	15	0.57
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	20	0.57
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	17	0.57
(1,310)	1:18:A:THR:H	1:18:A:THR:HG21	1	0.57
(1,310)	1:18:A:THR:H	1:18:A:THR:HG21	6	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:18:A:THR:HG22	1:20:A:LYS:HD2	18	0.57
(1,286)	1:18:A:THR:HA	1:30:A:TYR:HD1	9	0.57
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	1	0.57
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	11	0.57
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	15	0.57
(1,254)	1:14:A:ARG:HD2	1:14:A:ARG:HB2	17	0.57
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	3	0.57
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	11	0.57
(1,116)	1:63:A:PRO:HB2	1:63:A:PRO:HD2	18	0.57
(1,110)	1:5:A:PRO:HA	1:6:A:ASN:HB3	4	0.57
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	12	0.57
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	1	0.57
(1,61)	1:71:A:TYR:HE1	1:71:A:TYR:HA	7	0.57
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	7	0.57
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	15	0.57
(1,6)	1:7:A:PRO:HD2	1:21:A:LYS:HE3	12	0.57
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	18	0.56
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	3	0.56
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	17	0.56
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	10	0.56
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	11	0.56
(1,1854)	1:81:A:LYS:H	1:80:A:LEU:HG	13	0.56
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	8	0.56
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	13	0.56
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	4	0.56
(1,1807)	1:73:A:TYR:H	1:70:A:PRO:HB3	16	0.56
(1,1784)	1:67:A:CYS:H	1:66:A:LYS:HG2	6	0.56
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	12	0.56
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	9	0.56
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	16	0.56
(1,1740)	1:57:A:GLY:H	1:66:A:LYS:HB2	9	0.56
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	17	0.56
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	3	0.56
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	9	0.56
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	6	0.56
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	1	0.56
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	5	0.56
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	6	0.56
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	20	0.56
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	6	0.56
(1,1495)	1:2:A:VAL:HA	1:2:A:VAL:HG11	12	0.56
(1,1478)	1:18:A:THR:HG21	1:20:A:LYS:HB3	19	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	8	0.56
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	12	0.56
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	20	0.56
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	19	0.56
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	19	0.56
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	12	0.56
(1,1254)	1:78:A:CYS:HA	1:77:A:GLN:H	10	0.56
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	19	0.56
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	15	0.56
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	17	0.56
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD12	19	0.56
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	5	0.56
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	6	0.56
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	8	0.56
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	12	0.56
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	14	0.56
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	19	0.56
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	10	0.56
(1,1166)	1:71:A:TYR:HA	1:71:A:TYR:HD1	14	0.56
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	8	0.56
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	5	0.56
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	18	0.56
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	20	0.56
(1,1121)	1:70:A:PRO:HB2	1:69:A:CYS:HB2	16	0.56
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	1	0.56
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	17	0.56
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	10	0.56
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	17	0.56
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	12	0.56
(1,1001)	1:62:A:TYR:HA	1:63:A:PRO:HB3	15	0.56
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG12	4	0.56
(1,863)	1:56:A:CYS:H	1:55:A:THR:HB	6	0.56
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	2	0.56
(1,824)	1:51:A:LEU:HD21	1:51:A:LEU:H	17	0.56
(1,822)	1:51:A:LEU:HD21	1:56:A:CYS:HB3	11	0.56
(1,798)	1:50:A:CYS:HA	1:77:A:GLN:HA	11	0.56
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	2	0.56
(1,668)	1:40:A:CYS:HB2	1:35:A:TYR:HD1	13	0.56
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG23	19	0.56
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	19	0.56
(1,573)	1:73:A:TYR:HA	1:81:A:LYS:HG2	9	0.56
(1,562)	1:34:A:GLY:HA2	1:33:A:LYS:HB3	11	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	1	0.56
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	16	0.56
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	2	0.56
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	4	0.56
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	5	0.56
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	14	0.56
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	16	0.56
(1,490)	1:29:A:CYS:HA	1:20:A:LYS:HG2	14	0.56
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	3	0.56
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	6	0.56
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD22	1	0.56
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	7	0.56
(1,307)	1:18:A:THR:HG21	1:30:A:TYR:HE1	16	0.56
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	18	0.56
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	17	0.56
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	4	0.56
(1,212)	1:10:A:PRO:HA	1:9:A:SER:H	2	0.56
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	13	0.56
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	7	0.56
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	14	0.56
(1,183)	1:7:A:PRO:HG3	1:21:A:LYS:HG3	15	0.56
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	20	0.56
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	6	0.56
(1,116)	1:63:A:PRO:HB2	1:63:A:PRO:HD2	8	0.56
(1,116)	1:63:A:PRO:HB2	1:63:A:PRO:HD2	15	0.56
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	4	0.56
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	5	0.56
(1,61)	1:71:A:TYR:HE1	1:71:A:TYR:HA	11	0.56
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	6	0.56
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE2	3	0.56
(1,1860)	1:83:A:TYR:H	1:74:A:TYR:HD1	6	0.55
(1,1817)	1:74:A:TYR:H	1:73:A:TYR:HB2	19	0.55
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	6	0.55
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	14	0.55
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	14	0.55
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	6	0.55
(1,1748)	1:58:A:TYR:H	1:58:A:TYR:HB3	20	0.55
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	18	0.55
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	11	0.55
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	14	0.55
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	4	0.55
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	14	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1478)	1:18:A:THR:HG21	1:20:A:LYS:HB3	9	0.55
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	18	0.55
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	11	0.55
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	19	0.55
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	5	0.55
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	9	0.55
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	14	0.55
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	13	0.55
(1,1344)	1:81:A:LYS:HE2	1:83:A:TYR:HE1	8	0.55
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	13	0.55
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	16	0.55
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	18	0.55
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	8	0.55
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	16	0.55
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	18	0.55
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	1	0.55
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	10	0.55
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	11	0.55
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	4	0.55
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	10	0.55
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	8	0.55
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	19	0.55
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	18	0.55
(1,1177)	1:72:A:GLY:HA2	1:82:A:LYS:HB2	6	0.55
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	5	0.55
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	14	0.55
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	8	0.55
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	4	0.55
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	10	0.55
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	5	0.55
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	3	0.55
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	19	0.55
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	6	0.55
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	7	0.55
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	12	0.55
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	16	0.55
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	17	0.55
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	20	0.55
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	8	0.55
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	11	0.55
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	16	0.55
(1,965)	1:59:A:VAL:HG21	1:64:A:TYR:H	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG11	18	0.55
(1,891)	1:57:A:GLY:HA2	1:66:A:LYS:HB2	6	0.55
(1,827)	1:51:A:LEU:HD12	1:51:A:LEU:H	18	0.55
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	5	0.55
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	10	0.55
(1,736)	1:47:A:PRO:HA	1:47:A:PRO:HG3	19	0.55
(1,707)	1:44:A:ALA:HB2	1:58:A:TYR:HD1	15	0.55
(1,698)	1:44:A:ALA:HB3	1:65:A:TYR:HB2	16	0.55
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	17	0.55
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG23	15	0.55
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG22	1	0.55
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	3	0.55
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	4	0.55
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	3	0.55
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	14	0.55
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	6	0.55
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	8	0.55
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	15	0.55
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	18	0.55
(1,467)	1:66:A:LYS:HA	1:59:A:VAL:HG21	3	0.55
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	11	0.55
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	8	0.55
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	18	0.55
(1,310)	1:18:A:THR:H	1:18:A:THR:HG21	4	0.55
(1,307)	1:18:A:THR:HG22	1:30:A:TYR:HE1	18	0.55
(1,304)	1:18:A:THR:HG22	1:30:A:TYR:HB2	11	0.55
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	7	0.55
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	11	0.55
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	4	0.55
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	9	0.55
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	19	0.55
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	2	0.55
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	15	0.55
(1,84)	1:3:A:TYR:H	1:2:A:VAL:HG22	10	0.55
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	18	0.55
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	5	0.54
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	8	0.54
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	19	0.54
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	10	0.54
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	3	0.54
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	6	0.54
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	3	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	8	0.54
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	8	0.54
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	9	0.54
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	15	0.54
(1,1698)	1:44:A:ALA:H	1:58:A:TYR:HE1	12	0.54
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	2	0.54
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	8	0.54
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	17	0.54
(1,1508)	1:4:A:TYR:H	1:4:A:TYR:HD1	10	0.54
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	19	0.54
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	19	0.54
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	2	0.54
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	9	0.54
(1,1373)	1:72:A:GLY:HA2	1:82:A:LYS:HD2	3	0.54
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	2	0.54
(1,1350)	1:82:A:LYS:HA	1:82:A:LYS:HE2	19	0.54
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	17	0.54
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	1	0.54
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	2	0.54
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	4	0.54
(1,1246)	1:77:A:GLN:HA	1:77:A:GLN:HG2	5	0.54
(1,1246)	1:77:A:GLN:HA	1:77:A:GLN:HG2	11	0.54
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD12	17	0.54
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	17	0.54
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	18	0.54
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	1	0.54
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	14	0.54
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	16	0.54
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	17	0.54
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	18	0.54
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	19	0.54
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	3	0.54
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	13	0.54
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	7	0.54
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	3	0.54
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	17	0.54
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	2	0.54
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	11	0.54
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	9	0.54
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	19	0.54
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	9	0.54
(1,1084)	1:67:A:CYS:HA	1:68:A:SER:HB2	12	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG12	12	0.54
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	20	0.54
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	4	0.54
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	5	0.54
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	16	0.54
(1,828)	1:51:A:LEU:HD13	1:52:A:ASN:H	2	0.54
(1,828)	1:51:A:LEU:HD12	1:52:A:ASN:H	12	0.54
(1,828)	1:51:A:LEU:HD12	1:52:A:ASN:H	15	0.54
(1,827)	1:51:A:LEU:HD11	1:51:A:LEU:H	19	0.54
(1,824)	1:51:A:LEU:HD23	1:51:A:LEU:H	16	0.54
(1,822)	1:51:A:LEU:HD23	1:56:A:CYS:HB3	19	0.54
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	15	0.54
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	6	0.54
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	8	0.54
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	17	0.54
(1,713)	1:45:A:CYS:HA	1:56:A:CYS:HB3	5	0.54
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	18	0.54
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	16	0.54
(1,635)	1:38:A:LYS:HG3	1:38:A:LYS:HE2	13	0.54
(1,623)	1:38:A:LYS:HB3	1:38:A:LYS:HE2	9	0.54
(1,607)	1:36:A:THR:H	1:36:A:THR:HG22	13	0.54
(1,606)	1:44:A:ALA:H	1:36:A:THR:HG22	16	0.54
(1,599)	1:36:A:THR:HG21	1:64:A:TYR:HB3	12	0.54
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	20	0.54
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	2	0.54
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG23	11	0.54
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	5	0.54
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	18	0.54
(1,551)	1:33:A:LYS:HB3	1:33:A:LYS:HE2	8	0.54
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	2	0.54
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	3	0.54
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	17	0.54
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG11	14	0.54
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	2	0.54
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	5	0.54
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	8	0.54
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	11	0.54
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	20	0.54
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	12	0.54
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	3	0.54
(1,302)	1:18:A:THR:HG22	1:20:A:LYS:HD2	3	0.54
(1,302)	1:18:A:THR:HG23	1:20:A:LYS:HD2	13	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:18:A:THR:HG23	1:20:A:LYS:HD2	15	0.54
(1,262)	1:15:A:ASN:HB3	1:35:A:TYR:HD1	4	0.54
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	13	0.54
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	4	0.54
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	18	0.54
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	2	0.54
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG22	5	0.54
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	9	0.54
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	10	0.54
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	11	0.54
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	4	0.53
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	14	0.53
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	13	0.53
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	19	0.53
(1,1756)	1:59:A:VAL:H	1:66:A:LYS:H	6	0.53
(1,1698)	1:44:A:ALA:H	1:58:A:TYR:HE1	15	0.53
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	13	0.53
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	5	0.53
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	2	0.53
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	3	0.53
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	17	0.53
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	4	0.53
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	5	0.53
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	16	0.53
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	20	0.53
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD23	20	0.53
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	16	0.53
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	20	0.53
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	17	0.53
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	6	0.53
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	13	0.53
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	20	0.53
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	19	0.53
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	12	0.53
(1,1198)	1:74:A:TYR:HB2	1:74:A:TYR:HD1	16	0.53
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	2	0.53
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	6	0.53
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	1	0.53
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	14	0.53
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	14	0.53
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	19	0.53
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	16	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	13	0.53
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	10	0.53
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	18	0.53
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	1	0.53
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	20	0.53
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	3	0.53
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	5	0.53
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	17	0.53
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	19	0.53
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	10	0.53
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	18	0.53
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	13	0.53
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	14	0.53
(1,664)	1:40:A:CYS:HB2	1:31:A:CYS:HA	20	0.53
(1,641)	1:39:A:ASN:HA	1:29:A:CYS:HB3	17	0.53
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	1	0.53
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	8	0.53
(1,617)	1:38:A:LYS:HA	1:38:A:LYS:HE3	18	0.53
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	9	0.53
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG22	4	0.53
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	8	0.53
(1,551)	1:33:A:LYS:HB3	1:33:A:LYS:HE2	12	0.53
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	15	0.53
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	7	0.53
(1,528)	1:32:A:ARG:HB2	1:32:A:ARG:HD2	17	0.53
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	6	0.53
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	12	0.53
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	1	0.53
(1,333)	1:20:A:LYS:HB2	1:22:A:ARG:HD2	17	0.53
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG21	4	0.53
(1,308)	1:18:A:THR:HG22	1:30:A:TYR:HD1	11	0.53
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	11	0.53
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	17	0.53
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	4	0.53
(1,238)	1:13:A:CYS:HA	1:41:A:GLN:HB3	14	0.53
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	12	0.53
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	19	0.53
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	13	0.53
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	6	0.53
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	18	0.53
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	5	0.53
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	8	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:3:A:TYR:H	1:2:A:VAL:HA	12	0.53
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	18	0.53
(1,61)	1:71:A:TYR:HE1	1:71:A:TYR:HA	20	0.53
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	4	0.53
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	3	0.53
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	6	0.52
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	4	0.52
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	7	0.52
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	19	0.52
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	4	0.52
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	10	0.52
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	8	0.52
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	15	0.52
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	3	0.52
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	12	0.52
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD12	14	0.52
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	16	0.52
(1,1566)	1:21:A:LYS:H	1:21:A:LYS:HB2	18	0.52
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	18	0.52
(1,1500)	1:51:A:LEU:HD23	1:50:A:CYS:H	16	0.52
(1,1478)	1:18:A:THR:HG23	1:20:A:LYS:HB3	12	0.52
(1,1478)	1:18:A:THR:HG23	1:20:A:LYS:HB3	15	0.52
(1,1412)	1:67:A:CYS:HB3	1:50:A:CYS:H	11	0.52
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	8	0.52
(1,1392)	1:83:A:TYR:HA	1:82:A:LYS:H	19	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	1	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	2	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	3	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	6	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	7	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	8	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	9	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	10	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	11	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	12	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	13	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	14	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	17	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	18	0.52
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	19	0.52
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	19	0.52
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	20	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	3	0.52
(1,1342)	1:81:A:LYS:HD2	1:82:A:LYS:H	15	0.52
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD11	2	0.52
(1,1281)	1:79:A:GLN:HG2	1:80:A:LEU:HB2	9	0.52
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	5	0.52
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	16	0.52
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	8	0.52
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	5	0.52
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	10	0.52
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	12	0.52
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	7	0.52
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	1	0.52
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	20	0.52
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	2	0.52
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	7	0.52
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	19	0.52
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	14	0.52
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	12	0.52
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	17	0.52
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG11	15	0.52
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	19	0.52
(1,1043)	1:65:A:TYR:HA	1:65:A:TYR:HD1	15	0.52
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	6	0.52
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	13	0.52
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	16	0.52
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG13	13	0.52
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG11	14	0.52
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	11	0.52
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	11	0.52
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	8	0.52
(1,872)	1:55:A:THR:HG21	1:67:A:CYS:HA	1	0.52
(1,827)	1:51:A:LEU:HD12	1:51:A:LEU:H	12	0.52
(1,824)	1:51:A:LEU:HD22	1:51:A:LEU:H	11	0.52
(1,822)	1:51:A:LEU:HD23	1:56:A:CYS:HB3	17	0.52
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	16	0.52
(1,762)	1:48:A:ASN:HA	1:49:A:PRO:HB3	2	0.52
(1,762)	1:48:A:ASN:HA	1:49:A:PRO:HB3	5	0.52
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	3	0.52
(1,736)	1:47:A:PRO:HA	1:47:A:PRO:HG3	8	0.52
(1,736)	1:47:A:PRO:HA	1:47:A:PRO:HG3	9	0.52
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	2	0.52
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB2	14	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:46:A:PHE:H	1:44:A:ALA:HB1	19	0.52
(1,698)	1:44:A:ALA:HB2	1:65:A:TYR:HB2	20	0.52
(1,665)	1:40:A:CYS:HB3	1:31:A:CYS:HA	20	0.52
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	11	0.52
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	11	0.52
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	16	0.52
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	14	0.52
(1,635)	1:38:A:LYS:HG3	1:38:A:LYS:HE2	8	0.52
(1,635)	1:38:A:LYS:HG3	1:38:A:LYS:HE2	14	0.52
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG22	4	0.52
(1,588)	1:58:A:TYR:HB2	1:59:A:VAL:H	17	0.52
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	4	0.52
(1,555)	1:33:A:LYS:HE2	1:33:A:LYS:HG2	6	0.52
(1,555)	1:33:A:LYS:HE2	1:33:A:LYS:HG2	17	0.52
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	13	0.52
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	2	0.52
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	13	0.52
(1,488)	1:28:A:LYS:HE2	1:28:A:LYS:HA	20	0.52
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	8	0.52
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	13	0.52
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	4	0.52
(1,399)	1:22:A:ARG:HG2	1:28:A:LYS:H	6	0.52
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	16	0.52
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	11	0.52
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	7	0.52
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	2	0.52
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	9	0.52
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	1	0.52
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	5	0.52
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	2	0.52
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	8	0.52
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	16	0.52
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	2	0.52
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	17	0.52
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	5	0.52
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	17	0.52
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	13	0.52
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	10	0.52
(1,1857)	1:83:A:TYR:H	1:82:A:LYS:HG2	17	0.51
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	11	0.51
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	5	0.51
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	14	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	16	0.51
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	2	0.51
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	20	0.51
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	11	0.51
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	19	0.51
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	13	0.51
(1,1500)	1:51:A:LEU:HD21	1:50:A:CYS:H	1	0.51
(1,1490)	1:3:A:TYR:HB2	1:3:A:TYR:HE1	17	0.51
(1,1486)	1:7:A:PRO:HD3	1:6:A:ASN:HB3	10	0.51
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	1	0.51
(1,1413)	1:28:A:LYS:HA	1:28:A:LYS:HB2	6	0.51
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	5	0.51
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	13	0.51
(1,1403)	1:76:A:LYS:HA	1:75:A:GLY:HA2	15	0.51
(1,1388)	1:83:A:TYR:HB2	1:83:A:TYR:HA	15	0.51
(1,1386)	1:83:A:TYR:HA	1:82:A:LYS:HB2	6	0.51
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	9	0.51
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	15	0.51
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	18	0.51
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	8	0.51
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	15	0.51
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	13	0.51
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	15	0.51
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	1	0.51
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD22	5	0.51
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	8	0.51
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	17	0.51
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	16	0.51
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	14	0.51
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD13	4	0.51
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	5	0.51
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	16	0.51
(1,1097)	1:69:A:CYS:HB2	1:70:A:PRO:HG3	16	0.51
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	18	0.51
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	2	0.51
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	5	0.51
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	9	0.51
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	10	0.51
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG12	4	0.51
(1,948)	1:59:A:VAL:HG12	1:64:A:TYR:HA	6	0.51
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG12	19	0.51
(1,940)	1:59:A:VAL:HG11	1:66:A:LYS:HG2	4	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	1:50:A:CYS:H	1:49:A:PRO:HG3	12	0.51
(1,787)	1:49:A:PRO:HD3	1:48:A:ASN:HB3	8	0.51
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	16	0.51
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	8	0.51
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	11	0.51
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	6	0.51
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	11	0.51
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	6	0.51
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	4	0.51
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	15	0.51
(1,607)	1:36:A:THR:H	1:36:A:THR:HG21	7	0.51
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	12	0.51
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	14	0.51
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	15	0.51
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	5	0.51
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	19	0.51
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	6	0.51
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	3	0.51
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	5	0.51
(1,478)	1:66:A:LYS:HB2	1:66:A:LYS:HE2	3	0.51
(1,478)	1:66:A:LYS:HB2	1:66:A:LYS:HE2	17	0.51
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	18	0.51
(1,412)	1:24:A:LEU:H	1:24:A:LEU:HD23	4	0.51
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	7	0.51
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	10	0.51
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	8	0.51
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	16	0.51
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	2	0.51
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG23	12	0.51
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG23	13	0.51
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	18	0.51
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	11	0.51
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	12	0.51
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	9	0.51
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	12	0.51
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	14	0.51
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	4	0.51
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	15	0.51
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	7	0.51
(1,68)	1:83:A:TYR:HD1	1:83:A:TYR:HB3	16	0.51
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	3	0.51
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:35:A:TYR:HA	1:40:A:CYS:HA	4	0.51
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	9	0.5
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	20	0.5
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	1	0.5
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	13	0.5
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	13	0.5
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	8	0.5
(1,1857)	1:83:A:TYR:H	1:82:A:LYS:HG2	16	0.5
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	1	0.5
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	20	0.5
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	7	0.5
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	20	0.5
(1,1570)	1:82:A:LYS:H	1:82:A:LYS:HB2	6	0.5
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	7	0.5
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	1	0.5
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	13	0.5
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	15	0.5
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	7	0.5
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	2	0.5
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	6	0.5
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	7	0.5
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	8	0.5
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	9	0.5
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	11	0.5
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	13	0.5
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	17	0.5
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	18	0.5
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	19	0.5
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	1	0.5
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	6	0.5
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	5	0.5
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	15	0.5
(1,1252)	1:78:A:CYS:HA	1:77:A:GLN:HA	12	0.5
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	9	0.5
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	18	0.5
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD11	3	0.5
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	1	0.5
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	11	0.5
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	19	0.5
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	7	0.5
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	11	0.5
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	13	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	20	0.5
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	8	0.5
(1,1159)	1:70:A:PRO:HG3	1:55:A:THR:H	3	0.5
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	2	0.5
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	7	0.5
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	12	0.5
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	16	0.5
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	2	0.5
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	16	0.5
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	17	0.5
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	19	0.5
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	8	0.5
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	3	0.5
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	9	0.5
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	4	0.5
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	7	0.5
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG13	1	0.5
(1,940)	1:59:A:VAL:HG11	1:66:A:LYS:HG2	12	0.5
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	2	0.5
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	3	0.5
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	4	0.5
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	6	0.5
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	12	0.5
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	15	0.5
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	16	0.5
(1,906)	1:58:A:TYR:HA	1:65:A:TYR:HB2	6	0.5
(1,828)	1:51:A:LEU:HD11	1:52:A:ASN:H	20	0.5
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	6	0.5
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	2	0.5
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	5	0.5
(1,736)	1:47:A:PRO:HA	1:47:A:PRO:HG3	18	0.5
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	11	0.5
(1,703)	1:44:A:ALA:HB2	1:58:A:TYR:HA	6	0.5
(1,695)	1:44:A:ALA:HB3	1:45:A:CYS:HB3	3	0.5
(1,645)	1:39:A:ASN:HB3	1:41:A:GLN:HB3	2	0.5
(1,635)	1:38:A:LYS:HG3	1:38:A:LYS:HE2	3	0.5
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	3	0.5
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	9	0.5
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	10	0.5
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	17	0.5
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	19	0.5
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	5	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	3	0.5
(1,555)	1:33:A:LYS:HE2	1:33:A:LYS:HG2	20	0.5
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	11	0.5
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	11	0.5
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	4	0.5
(1,478)	1:66:A:LYS:HB2	1:66:A:LYS:HE2	12	0.5
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	20	0.5
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	3	0.5
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	17	0.5
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	17	0.5
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	4	0.5
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG21	9	0.5
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG21	10	0.5
(1,302)	1:18:A:THR:HG21	1:20:A:LYS:HD2	9	0.5
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	2	0.5
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	5	0.5
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	3	0.5
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	8	0.5
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	6	0.5
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	10	0.5
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	10	0.5
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	14	0.5
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	1	0.5
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	13	0.5
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	19	0.5
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	2	0.5
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	3	0.5
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	11	0.5
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	17	0.5
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	10	0.5
(1,43)	1:2:A:VAL:HG23	1:4:A:TYR:HD1	13	0.5
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	20	0.5
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	9	0.5
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	16	0.5
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE2	10	0.5
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	10	0.49
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	18	0.49
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	17	0.49
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	1	0.49
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	13	0.49
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	1	0.49
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	11	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	18	0.49
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	2	0.49
(1,1510)	1:6:A:ASN:H	1:5:A:PRO:HB2	15	0.49
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	8	0.49
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	9	0.49
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	14	0.49
(1,1478)	1:18:A:THR:HG23	1:20:A:LYS:HB3	13	0.49
(1,1454)	1:33:A:LYS:HG2	1:33:A:LYS:HE3	3	0.49
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	11	0.49
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	11	0.49
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	13	0.49
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	14	0.49
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	18	0.49
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	4	0.49
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	12	0.49
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	14	0.49
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	15	0.49
(1,1372)	1:82:A:LYS:HD2	1:82:A:LYS:HG2	20	0.49
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	12	0.49
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	8	0.49
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	18	0.49
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	1	0.49
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	15	0.49
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	5	0.49
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	2	0.49
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	4	0.49
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	9	0.49
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	5	0.49
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	9	0.49
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	10	0.49
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	9	0.49
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	11	0.49
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	8	0.49
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	15	0.49
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	5	0.49
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	7	0.49
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	12	0.49
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	20	0.49
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	12	0.49
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	9	0.49
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	14	0.49
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	8	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	5	0.49
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	8	0.49
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	9	0.49
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	13	0.49
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	17	0.49
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	18	0.49
(1,891)	1:57:A:GLY:HA2	1:66:A:LYS:HB2	1	0.49
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	14	0.49
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	9	0.49
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	14	0.49
(1,736)	1:47:A:PRO:HA	1:47:A:PRO:HG3	1	0.49
(1,736)	1:47:A:PRO:HA	1:47:A:PRO:HG3	3	0.49
(1,703)	1:44:A:ALA:HB1	1:58:A:TYR:HA	2	0.49
(1,695)	1:44:A:ALA:HB2	1:45:A:CYS:HB3	15	0.49
(1,695)	1:44:A:ALA:HB1	1:45:A:CYS:HB3	16	0.49
(1,660)	1:40:A:CYS:HB3	1:35:A:TYR:HB3	7	0.49
(1,660)	1:40:A:CYS:HB3	1:35:A:TYR:HB3	18	0.49
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	12	0.49
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	5	0.49
(1,641)	1:39:A:ASN:HA	1:29:A:CYS:HB3	2	0.49
(1,617)	1:38:A:LYS:HA	1:38:A:LYS:HE3	4	0.49
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	1	0.49
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	6	0.49
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	11	0.49
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	13	0.49
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	16	0.49
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG23	2	0.49
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	9	0.49
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	10	0.49
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	6	0.49
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	20	0.49
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	5	0.49
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	7	0.49
(1,488)	1:28:A:LYS:HE2	1:28:A:LYS:HA	12	0.49
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	18	0.49
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	7	0.49
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	14	0.49
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	3	0.49
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	5	0.49
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	7	0.49
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	13	0.49
(1,286)	1:18:A:THR:HA	1:30:A:TYR:HD1	11	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	13	0.49
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	4	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	1	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	2	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	4	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	5	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	7	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	12	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	14	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	16	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	17	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	18	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	19	0.49
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	20	0.49
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	14	0.49
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	2	0.49
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	4	0.49
(1,139)	1:70:A:PRO:HG3	1:73:A:TYR:HD1	11	0.49
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	10	0.49
(1,136)	1:5:A:PRO:HG2	1:5:A:PRO:HA	19	0.49
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	20	0.49
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	7	0.49
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	13	0.49
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	20	0.49
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	10	0.48
(1,1829)	1:76:A:LYS:H	1:76:A:LYS:HG3	7	0.48
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	14	0.48
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	8	0.48
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	9	0.48
(1,1666)	1:79:A:GLN:H	1:80:A:LEU:HD12	8	0.48
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	7	0.48
(1,1603)	1:29:A:CYS:H	1:28:A:LYS:HE3	8	0.48
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	20	0.48
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	7	0.48
(1,1351)	1:83:A:TYR:HB2	1:82:A:LYS:HA	7	0.48
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	9	0.48
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	12	0.48
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	14	0.48
(1,1195)	1:74:A:TYR:HB2	1:73:A:TYR:HA	3	0.48
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	12	0.48
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	19	0.48
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	1	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	1	0.48
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	1	0.48
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	19	0.48
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	11	0.48
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	19	0.48
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	4	0.48
(1,1050)	1:65:A:TYR:HB3	1:58:A:TYR:HA	6	0.48
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG12	13	0.48
(1,939)	1:59:A:VAL:HG12	1:66:A:LYS:HG3	1	0.48
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	3	0.48
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	7	0.48
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	10	0.48
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	14	0.48
(1,824)	1:51:A:LEU:HD22	1:51:A:LEU:H	10	0.48
(1,822)	1:51:A:LEU:HD22	1:56:A:CYS:HB3	9	0.48
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	10	0.48
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	12	0.48
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	13	0.48
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	8	0.48
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	7	0.48
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	19	0.48
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	9	0.48
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	18	0.48
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	8	0.48
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	6	0.48
(1,647)	1:39:A:ASN:HB2	1:41:A:GLN:HB3	6	0.48
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG22	13	0.48
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	4	0.48
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	7	0.48
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	18	0.48
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	20	0.48
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG23	5	0.48
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG22	13	0.48
(1,565)	1:34:A:GLY:HA3	1:35:A:TYR:HD1	18	0.48
(1,564)	1:34:A:GLY:HA3	1:58:A:TYR:HE1	19	0.48
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	1	0.48
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	7	0.48
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	20	0.48
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	8	0.48
(1,474)	1:66:A:LYS:HB2	1:59:A:VAL:HG21	6	0.48
(1,455)	1:27:A:TYR:HA	1:21:A:LYS:HB2	6	0.48
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	17	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	18	0.48
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	11	0.48
(1,302)	1:18:A:THR:HG22	1:20:A:LYS:HD2	11	0.48
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	10	0.48
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	19	0.48
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	10	0.48
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	19	0.48
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	20	0.48
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	2	0.48
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	9	0.48
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	13	0.48
(1,202)	1:26:A:SER:HB2	1:26:A:SER:HA	15	0.48
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	12	0.48
(1,183)	1:7:A:PRO:HG3	1:21:A:LYS:HG3	11	0.48
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	1	0.48
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	8	0.48
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	13	0.48
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	11	0.48
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	5	0.48
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	9	0.48
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	4	0.48
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	4	0.48
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	5	0.48
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	2	0.48
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	3	0.48
(1,43)	1:2:A:VAL:HG21	1:4:A:TYR:HD1	17	0.48
(1,36)	1:83:A:TYR:H	1:82:A:LYS:HB3	7	0.48
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	17	0.48
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	16	0.47
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	13	0.47
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	12	0.47
(1,1804)	1:72:A:GLY:H	1:71:A:TYR:HD1	19	0.47
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	12	0.47
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	19	0.47
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	4	0.47
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	11	0.47
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	20	0.47
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD13	3	0.47
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	10	0.47
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	15	0.47
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	16	0.47
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	8	0.47
(1,1402)	1:80:A:LEU:HD21	1:75:A:GLY:HA3	9	0.47
(1,1381)	1:82:A:LYS:HG2	1:74:A:TYR:HE1	6	0.47
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	14	0.47
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	14	0.47
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	14	0.47
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	14	0.47
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	10	0.47
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	10	0.47
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	10	0.47
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	11	0.47
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	11	0.47
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	16	0.47
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	17	0.47
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	17	0.47
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	3	0.47
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	6	0.47
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	7	0.47
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	10	0.47
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	14	0.47
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	19	0.47
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	3	0.47
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG11	18	0.47
(1,940)	1:59:A:VAL:HG11	1:66:A:LYS:HG2	15	0.47
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	20	0.47
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	1	0.47
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	11	0.47
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	19	0.47
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	9	0.47
(1,869)	1:55:A:THR:HG22	1:68:A:SER:HB3	18	0.47
(1,841)	1:53:A:GLY:HA3	1:70:A:PRO:HG2	3	0.47
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	10	0.47
(1,822)	1:51:A:LEU:HD21	1:56:A:CYS:HB3	3	0.47
(1,815)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	16	0.47
(1,798)	1:50:A:CYS:HA	1:77:A:GLN:HA	15	0.47
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	17	0.47
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	1	0.47
(1,754)	1:47:A:PRO:HD3	1:46:A:PHE:HD1	19	0.47
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	1	0.47
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	8	0.47
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	9	0.47
(1,707)	1:44:A:ALA:HB2	1:58:A:TYR:HD1	13	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:44:A:ALA:HB2	1:65:A:TYR:HA	19	0.47
(1,695)	1:44:A:ALA:HB2	1:45:A:CYS:HB3	13	0.47
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	14	0.47
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	1	0.47
(1,623)	1:38:A:LYS:HB3	1:38:A:LYS:HE2	7	0.47
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	8	0.47
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	2	0.47
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	5	0.47
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	12	0.47
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	19	0.47
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	19	0.47
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	11	0.47
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	1	0.47
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	8	0.47
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	3	0.47
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	19	0.47
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	1	0.47
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	8	0.47
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	19	0.47
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	11	0.47
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	4	0.47
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	1	0.47
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	8	0.47
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	20	0.47
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	10	0.47
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	1	0.47
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	15	0.47
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	20	0.47
(1,183)	1:7:A:PRO:HG3	1:21:A:LYS:HG3	5	0.47
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	12	0.47
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	13	0.47
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	10	0.47
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	11	0.47
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	12	0.47
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	14	0.47
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	18	0.47
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	8	0.47
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	6	0.47
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	9	0.47
(1,1805)	1:73:A:TYR:H	1:82:A:LYS:HG2	5	0.46
(1,1804)	1:72:A:GLY:H	1:71:A:TYR:HD1	3	0.46
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	18	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	9	0.46
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	11	0.46
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	13	0.46
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	14	0.46
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	19	0.46
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	6	0.46
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	7	0.46
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	18	0.46
(1,1620)	1:31:A:CYS:H	1:18:A:THR:HB	11	0.46
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	20	0.46
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	8	0.46
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	3	0.46
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	12	0.46
(1,1478)	1:18:A:THR:HG22	1:20:A:LYS:HB3	7	0.46
(1,1461)	1:28:A:LYS:HB3	1:30:A:TYR:HE1	2	0.46
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	7	0.46
(1,1417)	1:63:A:PRO:HB2	1:64:A:TYR:HD1	19	0.46
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	13	0.46
(1,1368)	1:82:A:LYS:HB2	1:83:A:TYR:HD1	6	0.46
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	19	0.46
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD11	4	0.46
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD12	20	0.46
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	14	0.46
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	19	0.46
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	4	0.46
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	14	0.46
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	18	0.46
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	19	0.46
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	2	0.46
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	19	0.46
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	20	0.46
(1,1085)	1:68:A:SER:HB3	1:55:A:THR:H	20	0.46
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	3	0.46
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	11	0.46
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	17	0.46
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	1	0.46
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	1	0.46
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	5	0.46
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	6	0.46
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG11	16	0.46
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG12	7	0.46
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	11	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	13	0.46
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	12	0.46
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	7	0.46
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	20	0.46
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	14	0.46
(1,623)	1:38:A:LYS:HB3	1:38:A:LYS:HE2	15	0.46
(1,608)	1:37:A:GLY:HA3	1:36:A:THR:HG21	12	0.46
(1,600)	1:36:A:THR:HG22	1:64:A:TYR:HB2	17	0.46
(1,599)	1:36:A:THR:HG23	1:64:A:TYR:HB3	13	0.46
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	5	0.46
(1,584)	1:80:A:LEU:H	1:73:A:TYR:HA	11	0.46
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	17	0.46
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	10	0.46
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	5	0.46
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	9	0.46
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	1	0.46
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	4	0.46
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	16	0.46
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	1	0.46
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	15	0.46
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	13	0.46
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	17	0.46
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	15	0.46
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	7	0.46
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	16	0.46
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	2	0.46
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	14	0.46
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	18	0.46
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	8	0.46
(1,297)	1:18:A:THR:HB	1:30:A:TYR:HE1	16	0.46
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	5	0.46
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	6	0.46
(1,249)	1:13:A:CYS:HB2	1:11:A:TYR:HD1	7	0.46
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	14	0.46
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	18	0.46
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	3	0.46
(1,212)	1:10:A:PRO:HA	1:9:A:SER:H	8	0.46
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	5	0.46
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	7	0.46
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	1	0.46
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	17	0.46
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	13	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	17	0.46
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	20	0.46
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	6	0.46
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	15	0.46
(1,83)	1:2:A:VAL:HG22	1:4:A:TYR:HE1	1	0.46
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	15	0.46
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	2	0.46
(1,38)	1:82:A:LYS:H	1:74:A:TYR:HE1	16	0.46
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	19	0.46
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	18	0.46
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	16	0.46
(1,1886)	1:22:A:ARG:H	1:27:A:TYR:HD1	17	0.45
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	2	0.45
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	3	0.45
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	11	0.45
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	3	0.45
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	13	0.45
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	5	0.45
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	17	0.45
(1,1703)	1:45:A:CYS:H	1:58:A:TYR:HD1	3	0.45
(1,1620)	1:31:A:CYS:H	1:18:A:THR:HB	5	0.45
(1,1591)	1:26:A:SER:H	1:25:A:TYR:HE1	15	0.45
(1,1478)	1:18:A:THR:HG21	1:20:A:LYS:HB3	16	0.45
(1,1469)	1:22:A:ARG:HB3	1:22:A:ARG:HD2	3	0.45
(1,1469)	1:22:A:ARG:HB3	1:22:A:ARG:HD2	5	0.45
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	18	0.45
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	12	0.45
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	7	0.45
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD22	15	0.45
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD13	14	0.45
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	6	0.45
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	19	0.45
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	2	0.45
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	18	0.45
(1,1199)	1:74:A:TYR:HB3	1:74:A:TYR:HD1	15	0.45
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	17	0.45
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	17	0.45
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	1	0.45
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	7	0.45
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	9	0.45
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	13	0.45
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	18	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	20	0.45
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	9	0.45
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG11	17	0.45
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	15	0.45
(1,919)	1:58:A:TYR:HB2	1:58:A:TYR:HD1	20	0.45
(1,822)	1:51:A:LEU:HD23	1:56:A:CYS:HB3	4	0.45
(1,794)	1:50:A:CYS:HA	1:77:A:GLN:HG2	11	0.45
(1,792)	1:50:A:CYS:HA	1:77:A:GLN:HG3	17	0.45
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	6	0.45
(1,741)	1:47:A:PRO:HA	1:46:A:PHE:HD1	20	0.45
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	7	0.45
(1,729)	1:46:A:PHE:HA	1:46:A:PHE:HD1	11	0.45
(1,715)	1:45:A:CYS:HA	1:43:A:ASN:HB2	8	0.45
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	5	0.45
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	1	0.45
(1,636)	1:38:A:LYS:HG3	1:38:A:LYS:HA	3	0.45
(1,599)	1:36:A:THR:HG22	1:64:A:TYR:HB3	10	0.45
(1,585)	1:36:A:THR:H	1:35:A:TYR:HA	2	0.45
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	18	0.45
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	8	0.45
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	13	0.45
(1,484)	1:28:A:LYS:HB3	1:21:A:LYS:HA	7	0.45
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	3	0.45
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	12	0.45
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	2	0.45
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	2	0.45
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD11	12	0.45
(1,386)	1:22:A:ARG:HD2	1:22:A:ARG:HG2	17	0.45
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	12	0.45
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	13	0.45
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	15	0.45
(1,374)	1:21:A:LYS:HG2	1:21:A:LYS:H	11	0.45
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	9	0.45
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG23	15	0.45
(1,270)	1:17:A:GLY:HA2	1:32:A:ARG:HG2	15	0.45
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	5	0.45
(1,212)	1:10:A:PRO:HA	1:9:A:SER:H	10	0.45
(1,212)	1:10:A:PRO:HA	1:9:A:SER:H	17	0.45
(1,204)	1:26:A:SER:HB2	1:27:A:TYR:HD1	20	0.45
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	10	0.45
(1,134)	1:4:A:TYR:H	1:5:A:PRO:HD3	19	0.45
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	7	0.45
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	7	0.45
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	6	0.45
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	3	0.45
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	8	0.45
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	15	0.44
(1,1829)	1:76:A:LYS:H	1:76:A:LYS:HG3	12	0.44
(1,1810)	1:73:A:TYR:H	1:81:A:LYS:HA	9	0.44
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	1	0.44
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	5	0.44
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	8	0.44
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	10	0.44
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	17	0.44
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	8	0.44
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	16	0.44
(1,1749)	1:58:A:TYR:H	1:58:A:TYR:HD1	6	0.44
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	16	0.44
(1,1740)	1:57:A:GLY:H	1:66:A:LYS:HB2	18	0.44
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	8	0.44
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	9	0.44
(1,1709)	1:46:A:PHE:H	1:46:A:PHE:HD1	17	0.44
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	12	0.44
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	18	0.44
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	10	0.44
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	1	0.44
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	8	0.44
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	17	0.44
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	10	0.44
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	1	0.44
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	5	0.44
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	12	0.44
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	13	0.44
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	19	0.44
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	4	0.44
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	8	0.44
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	11	0.44
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	12	0.44
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	17	0.44
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	18	0.44
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	4	0.44
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	19	0.44
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	15	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	17	0.44
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	3	0.44
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	5	0.44
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	12	0.44
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	8	0.44
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	7	0.44
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	8	0.44
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	9	0.44
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	17	0.44
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	1	0.44
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	2	0.44
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	6	0.44
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	8	0.44
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	12	0.44
(1,1036)	1:59:A:VAL:HG13	1:65:A:TYR:HA	13	0.44
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	19	0.44
(1,955)	1:61:A:GLY:H	1:59:A:VAL:HG13	20	0.44
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	10	0.44
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	19	0.44
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	13	0.44
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	16	0.44
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	18	0.44
(1,824)	1:51:A:LEU:HD23	1:51:A:LEU:H	14	0.44
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	1	0.44
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	4	0.44
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	20	0.44
(1,707)	1:44:A:ALA:HB3	1:58:A:TYR:HD1	3	0.44
(1,695)	1:44:A:ALA:HB1	1:45:A:CYS:HB3	2	0.44
(1,695)	1:44:A:ALA:HB3	1:45:A:CYS:HB3	9	0.44
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	18	0.44
(1,636)	1:38:A:LYS:HG3	1:38:A:LYS:HA	12	0.44
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	19	0.44
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	17	0.44
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	18	0.44
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	2	0.44
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	2	0.44
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	3	0.44
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	19	0.44
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	3	0.44
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	12	0.44
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD13	5	0.44
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	9	0.44
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	1	0.44
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG21	19	0.44
(1,302)	1:18:A:THR:HG23	1:20:A:LYS:HD2	12	0.44
(1,302)	1:18:A:THR:HG21	1:20:A:LYS:HD2	19	0.44
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	1	0.44
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	8	0.44
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	4	0.44
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	10	0.44
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	9	0.44
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	17	0.44
(1,212)	1:10:A:PRO:HA	1:9:A:SER:H	18	0.44
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	2	0.44
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	4	0.44
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	8	0.44
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	2	0.44
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	16	0.44
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	17	0.44
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	19	0.44
(1,61)	1:71:A:TYR:HE1	1:71:A:TYR:HA	9	0.44
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	16	0.44
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	7	0.44
(1,29)	1:32:A:ARG:H	1:32:A:ARG:HB3	9	0.44
(1,15)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	15	0.44
(1,1886)	1:22:A:ARG:H	1:27:A:TYR:HD1	20	0.43
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	12	0.43
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	17	0.43
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	13	0.43
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	17	0.43
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	4	0.43
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	6	0.43
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	9	0.43
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	12	0.43
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	19	0.43
(1,1776)	1:65:A:TYR:H	1:59:A:VAL:HB	11	0.43
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	4	0.43
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	7	0.43
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	10	0.43
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	15	0.43
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	3	0.43
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	19	0.43
(1,1667)	1:79:A:GLN:H	1:80:A:LEU:HD21	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1651)	1:36:A:THR:H	1:42:A:TYR:H	8	0.43
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	9	0.43
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	9	0.43
(1,1529)	1:15:A:ASN:H	1:14:A:ARG:HD2	2	0.43
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	2	0.43
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	13	0.43
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	5	0.43
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	4	0.43
(1,1436)	1:44:A:ALA:HB3	1:58:A:TYR:HE1	9	0.43
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	3	0.43
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	16	0.43
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	4	0.43
(1,1319)	1:79:A:GLN:HG3	1:80:A:LEU:HD21	2	0.43
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	14	0.43
(1,1292)	1:80:A:LEU:HA	1:79:A:GLN:HG3	7	0.43
(1,1288)	1:80:A:LEU:H	1:79:A:GLN:HG3	1	0.43
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	4	0.43
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	18	0.43
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	9	0.43
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	1	0.43
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	2	0.43
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	17	0.43
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	4	0.43
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	9	0.43
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	5	0.43
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	20	0.43
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	6	0.43
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	3	0.43
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	13	0.43
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	18	0.43
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	6	0.43
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	13	0.43
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	7	0.43
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	10	0.43
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	15	0.43
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	19	0.43
(1,1036)	1:59:A:VAL:HG13	1:65:A:TYR:HA	12	0.43
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	10	0.43
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	13	0.43
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	4	0.43
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	7	0.43
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:51:A:LEU:HD22	1:51:A:LEU:H	13	0.43
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	19	0.43
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	15	0.43
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	6	0.43
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	9	0.43
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	13	0.43
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	15	0.43
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	9	0.43
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	12	0.43
(1,636)	1:38:A:LYS:HG3	1:38:A:LYS:HA	15	0.43
(1,636)	1:38:A:LYS:HG3	1:38:A:LYS:HA	16	0.43
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	1	0.43
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	3	0.43
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	8	0.43
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	9	0.43
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	16	0.43
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	13	0.43
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	6	0.43
(1,569)	1:34:A:GLY:HA2	1:58:A:TYR:HD1	14	0.43
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	15	0.43
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	6	0.43
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	6	0.43
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	13	0.43
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	15	0.43
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	3	0.43
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	3	0.43
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	5	0.43
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	6	0.43
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	8	0.43
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	9	0.43
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	10	0.43
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	12	0.43
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	13	0.43
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	15	0.43
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	16	0.43
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	1	0.43
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	14	0.43
(1,407)	1:24:A:LEU:H	1:23:A:GLY:HA2	20	0.43
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	10	0.43
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	17	0.43
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	15	0.43
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	8	0.43
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	10	0.43
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	13	0.43
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	17	0.43
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	20	0.43
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	16	0.43
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	8	0.43
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	11	0.43
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	7	0.43
(1,138)	1:5:A:PRO:HG2	1:3:A:TYR:HE1	6	0.43
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	1	0.43
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	4	0.43
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	10	0.43
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	12	0.43
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	13	0.43
(1,92)	1:3:A:TYR:HB3	1:2:A:VAL:HA	18	0.43
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	14	0.43
(1,60)	1:71:A:TYR:HD1	1:71:A:TYR:HB3	2	0.43
(1,60)	1:71:A:TYR:HD1	1:71:A:TYR:HB3	4	0.43
(1,60)	1:71:A:TYR:HD1	1:71:A:TYR:HB3	12	0.43
(1,60)	1:71:A:TYR:HD1	1:71:A:TYR:HB3	17	0.43
(1,38)	1:82:A:LYS:H	1:74:A:TYR:HE1	12	0.43
(1,24)	1:78:A:CYS:HB3	1:70:A:PRO:HD3	9	0.43
(1,24)	1:78:A:CYS:HB3	1:70:A:PRO:HD3	11	0.43
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	3	0.42
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	1	0.42
(1,1811)	1:73:A:TYR:H	1:73:A:TYR:HE1	17	0.42
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	7	0.42
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	16	0.42
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	20	0.42
(1,1791)	1:68:A:SER:H	1:67:A:CYS:HB2	12	0.42
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	1	0.42
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	19	0.42
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	17	0.42
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	7	0.42
(1,1676)	1:79:A:GLN:H	1:75:A:GLY:HA2	10	0.42
(1,1671)	1:41:A:GLN:H	1:39:A:ASN:HB3	17	0.42
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	7	0.42
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	7	0.42
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	20	0.42
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	2	0.42
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	16	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	1:44:A:ALA:HB3	1:58:A:TYR:HE1	3	0.42
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	16	0.42
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	6	0.42
(1,1374)	1:82:A:LYS:HA	1:82:A:LYS:HD2	6	0.42
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	7	0.42
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	3	0.42
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	14	0.42
(1,1243)	1:77:A:GLN:HG2	1:49:A:PRO:HB3	20	0.42
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	14	0.42
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	3	0.42
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	5	0.42
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	14	0.42
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	19	0.42
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	16	0.42
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	17	0.42
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	14	0.42
(1,1088)	1:69:A:CYS:HA	1:70:A:PRO:HB2	15	0.42
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	20	0.42
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	1	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	1	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	2	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	3	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	5	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	8	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	9	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	10	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	12	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	13	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	15	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	16	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	17	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	19	0.42
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	20	0.42
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	15	0.42
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	4	0.42
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	16	0.42
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	10	0.42
(1,944)	1:58:A:TYR:HB3	1:59:A:VAL:HG11	9	0.42
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	4	0.42
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	7	0.42
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	15	0.42
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	13	0.42
(1,838)	1:53:A:GLY:HA2	1:70:A:PRO:HG3	15	0.42
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	8	0.42
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	12	0.42
(1,822)	1:51:A:LEU:HD23	1:56:A:CYS:HB3	6	0.42
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	14	0.42
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	19	0.42
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	4	0.42
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	11	0.42
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	12	0.42
(1,703)	1:44:A:ALA:HB2	1:58:A:TYR:HA	11	0.42
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	16	0.42
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	2	0.42
(1,636)	1:38:A:LYS:HG3	1:38:A:LYS:HA	5	0.42
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	12	0.42
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	14	0.42
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	15	0.42
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	17	0.42
(1,604)	1:35:A:TYR:H	1:36:A:THR:HG21	7	0.42
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	9	0.42
(1,588)	1:58:A:TYR:HB2	1:59:A:VAL:H	11	0.42
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	14	0.42
(1,573)	1:73:A:TYR:HA	1:81:A:LYS:HG2	7	0.42
(1,543)	1:32:A:ARG:HA	1:33:A:LYS:HA	8	0.42
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	10	0.42
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	14	0.42
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	11	0.42
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	17	0.42
(1,487)	1:28:A:LYS:HE2	1:28:A:LYS:HD2	11	0.42
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	9	0.42
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	16	0.42
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	20	0.42
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	20	0.42
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	6	0.42
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	15	0.42
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	9	0.42
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	17	0.42
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	4	0.42
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	12	0.42
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	5	0.42
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	20	0.42
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	20	0.42
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	8	0.42
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	16	0.42
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	1	0.42
(1,209)	1:10:A:PRO:HA	1:11:A:TYR:HB2	8	0.42
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	4	0.42
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	12	0.42
(1,117)	1:5:A:PRO:HB2	1:5:A:PRO:HD2	19	0.42
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	9	0.42
(1,60)	1:71:A:TYR:HD1	1:71:A:TYR:HB3	1	0.42
(1,60)	1:71:A:TYR:HD1	1:71:A:TYR:HB3	8	0.42
(1,60)	1:71:A:TYR:HD1	1:71:A:TYR:HB3	13	0.42
(1,60)	1:71:A:TYR:HD1	1:71:A:TYR:HB3	16	0.42
(1,60)	1:71:A:TYR:HD1	1:71:A:TYR:HB3	18	0.42
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	13	0.42
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	20	0.41
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	14	0.41
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	15	0.41
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	7	0.41
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	8	0.41
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	12	0.41
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	2	0.41
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	18	0.41
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	6	0.41
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	17	0.41
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	20	0.41
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	11	0.41
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	8	0.41
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	1	0.41
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	3	0.41
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	1	0.41
(1,1620)	1:31:A:CYS:H	1:18:A:THR:HB	20	0.41
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	12	0.41
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	18	0.41
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	5	0.41
(1,1478)	1:18:A:THR:HG23	1:20:A:LYS:HB3	20	0.41
(1,1477)	1:18:A:THR:HG22	1:19:A:CYS:HB3	8	0.41
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	1	0.41
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	2	0.41
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	7	0.41
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	1	0.41
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	6	0.41
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	7	0.41
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	7	0.41
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	9	0.41
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	16	0.41
(1,1191)	1:73:A:TYR:HB3	1:70:A:PRO:HD3	19	0.41
(1,1125)	1:70:A:PRO:HB2	1:54:A:GLY:HA3	11	0.41
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	4	0.41
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	17	0.41
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	6	0.41
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	10	0.41
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	16	0.41
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	4	0.41
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	11	0.41
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	14	0.41
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	18	0.41
(1,1056)	1:66:A:LYS:H	1:65:A:TYR:HB2	9	0.41
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	1	0.41
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	2	0.41
(1,1047)	1:58:A:TYR:H	1:65:A:TYR:HA	12	0.41
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	3	0.41
(1,1016)	1:64:A:TYR:H	1:63:A:PRO:HG2	20	0.41
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	9	0.41
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	6	0.41
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG11	11	0.41
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	1	0.41
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	1	0.41
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	3	0.41
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	4	0.41
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	19	0.41
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	8	0.41
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	9	0.41
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	2	0.41
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	2	0.41
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	17	0.41
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	5	0.41
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	4	0.41
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	10	0.41
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	20	0.41
(1,603)	1:36:A:THR:HG23	1:42:A:TYR:HA	3	0.41
(1,597)	1:36:A:THR:HG21	1:42:A:TYR:HB3	15	0.41
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:58:A:TYR:HB2	1:59:A:VAL:H	13	0.41
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	11	0.41
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	5	0.41
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	6	0.41
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	5	0.41
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	4	0.41
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	18	0.41
(1,477)	1:28:A:LYS:HB2	1:28:A:LYS:HE3	4	0.41
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	2	0.41
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	12	0.41
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	14	0.41
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	15	0.41
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	2	0.41
(1,344)	1:18:A:THR:HG23	1:20:A:LYS:HE2	3	0.41
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	14	0.41
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG23	20	0.41
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	3	0.41
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	11	0.41
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	15	0.41
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	7	0.41
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	12	0.41
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	3	0.41
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	5	0.41
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	7	0.41
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	12	0.41
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	15	0.41
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	17	0.41
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	18	0.41
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	20	0.41
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	15	0.41
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	1	0.41
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	11	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	1	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	2	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	3	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	4	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	5	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	7	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	8	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	9	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	10	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	12	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	13	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	18	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	19	0.41
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	20	0.41
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	12	0.41
(1,60)	1:71:A:TYR:HD1	1:71:A:TYR:HB3	15	0.41
(1,38)	1:82:A:LYS:H	1:74:A:TYR:HE1	8	0.41
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	6	0.41
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	7	0.4
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	10	0.4
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	20	0.4
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	10	0.4
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	5	0.4
(1,1829)	1:76:A:LYS:H	1:76:A:LYS:HG3	4	0.4
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	14	0.4
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	6	0.4
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	2	0.4
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	3	0.4
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	16	0.4
(1,1767)	1:62:A:TYR:H	1:62:A:TYR:HB3	18	0.4
(1,1745)	1:57:A:GLY:H	1:65:A:TYR:HD1	19	0.4
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	1	0.4
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	15	0.4
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	9	0.4
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	19	0.4
(1,1684)	1:42:A:TYR:H	1:39:A:ASN:HB2	16	0.4
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	16	0.4
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	13	0.4
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	14	0.4
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	5	0.4
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	10	0.4
(1,1486)	1:7:A:PRO:HD3	1:6:A:ASN:HB3	4	0.4
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	8	0.4
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	7	0.4
(1,1377)	1:82:A:LYS:HE2	1:82:A:LYS:HG2	13	0.4
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	9	0.4
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	14	0.4
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	15	0.4
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	2	0.4
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	11	0.4
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	10	0.4
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	18	0.4
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	20	0.4
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	7	0.4
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	10	0.4
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	18	0.4
(1,1182)	1:72:A:GLY:HA2	1:71:A:TYR:HD1	2	0.4
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	14	0.4
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	20	0.4
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	9	0.4
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	3	0.4
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	15	0.4
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	14	0.4
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	11	0.4
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	2	0.4
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	3	0.4
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	7	0.4
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	8	0.4
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	9	0.4
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	11	0.4
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	14	0.4
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	15	0.4
(1,1041)	1:65:A:TYR:HA	1:66:A:LYS:HA	5	0.4
(1,960)	1:59:A:VAL:HG23	1:60:A:TYR:HB2	10	0.4
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG11	6	0.4
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG12	8	0.4
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	12	0.4
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	1	0.4
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	12	0.4
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	1	0.4
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	17	0.4
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	8	0.4
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	19	0.4
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	4	0.4
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	1	0.4
(1,736)	1:47:A:PRO:HA	1:47:A:PRO:HG3	11	0.4
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	2	0.4
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	3	0.4
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	15	0.4
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	11	0.4
(1,641)	1:39:A:ASN:HA	1:29:A:CYS:HB3	8	0.4
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	2	0.4
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	7	0.4
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	18	0.4
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	18	0.4
(1,575)	1:73:A:TYR:HA	1:81:A:LYS:HB3	15	0.4
(1,561)	1:34:A:GLY:HA3	1:33:A:LYS:HB3	12	0.4
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	9	0.4
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	17	0.4
(1,533)	1:32:A:ARG:HD2	1:31:A:CYS:H	14	0.4
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	20	0.4
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	2	0.4
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	10	0.4
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	5	0.4
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	5	0.4
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	7	0.4
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	19	0.4
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD22	19	0.4
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	6	0.4
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	8	0.4
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	19	0.4
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	12	0.4
(1,344)	1:18:A:THR:HG22	1:20:A:LYS:HE2	9	0.4
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	3	0.4
(1,304)	1:18:A:THR:HG22	1:30:A:TYR:HB2	18	0.4
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	13	0.4
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	3	0.4
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	5	0.4
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	19	0.4
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	3	0.4
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	18	0.4
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	3	0.4
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	1	0.4
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	9	0.4
(1,210)	1:10:A:PRO:HA	1:10:A:PRO:HD2	14	0.4
(1,181)	1:7:A:PRO:HG2	1:27:A:TYR:HA	3	0.4
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	4	0.4
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	14	0.4
(1,132)	1:5:A:PRO:HD3	1:4:A:TYR:HB3	12	0.4
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	11	0.4
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	1	0.4
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	2	0.4
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	5	0.4
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	20	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	6	0.4
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	11	0.4
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	14	0.4
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	15	0.4
(1,87)	1:3:A:TYR:HA	1:3:A:TYR:HB3	16	0.4
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	1	0.4
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	12	0.4
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	13	0.4
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	11	0.4
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	3	0.4
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	7	0.39
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	19	0.39
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	3	0.39
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	11	0.39
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	9	0.39
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	15	0.39
(1,1740)	1:57:A:GLY:H	1:66:A:LYS:HB2	20	0.39
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	18	0.39
(1,1698)	1:44:A:ALA:H	1:58:A:TYR:HE1	9	0.39
(1,1666)	1:79:A:GLN:H	1:80:A:LEU:HD12	10	0.39
(1,1658)	1:39:A:ASN:H	1:41:A:GLN:H	13	0.39
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	19	0.39
(1,1636)	1:34:A:GLY:H	1:35:A:TYR:HD1	17	0.39
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	18	0.39
(1,1580)	1:24:A:LEU:H	1:25:A:TYR:HD1	15	0.39
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	3	0.39
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	16	0.39
(1,1500)	1:51:A:LEU:HD23	1:50:A:CYS:H	8	0.39
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	17	0.39
(1,1477)	1:18:A:THR:HG22	1:19:A:CYS:HB3	2	0.39
(1,1437)	1:44:A:ALA:HB2	1:36:A:THR:HG23	2	0.39
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	3	0.39
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	1	0.39
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	3	0.39
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	19	0.39
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	16	0.39
(1,1250)	1:78:A:CYS:HA	1:80:A:LEU:HB2	8	0.39
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	6	0.39
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	4	0.39
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	8	0.39
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	11	0.39
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	16	0.39
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	7	0.39
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	3	0.39
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	14	0.39
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	17	0.39
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	19	0.39
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	3	0.39
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	6	0.39
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	8	0.39
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	13	0.39
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	20	0.39
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	9	0.39
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	13	0.39
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	15	0.39
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	5	0.39
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	15	0.39
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	9	0.39
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	10	0.39
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	15	0.39
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	4	0.39
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	5	0.39
(1,1067)	1:66:A:LYS:HB3	1:66:A:LYS:HG3	7	0.39
(1,1036)	1:59:A:VAL:HG13	1:65:A:TYR:HA	15	0.39
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	4	0.39
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	4	0.39
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	7	0.39
(1,983)	1:62:A:TYR:HA	1:59:A:VAL:HG13	14	0.39
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	16	0.39
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	1	0.39
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	5	0.39
(1,891)	1:57:A:GLY:HA2	1:66:A:LYS:HB2	9	0.39
(1,802)	1:50:A:CYS:H	1:50:A:CYS:HB2	11	0.39
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	16	0.39
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	3	0.39
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	18	0.39
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	5	0.39
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	10	0.39
(1,707)	1:44:A:ALA:HB2	1:58:A:TYR:HD1	19	0.39
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	10	0.39
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	9	0.39
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	20	0.39
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,625)	1:38:A:LYS:H	1:38:A:LYS:HB3	11	0.39
(1,588)	1:58:A:TYR:HB2	1:59:A:VAL:H	5	0.39
(1,588)	1:58:A:TYR:HB2	1:59:A:VAL:H	14	0.39
(1,550)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	6	0.39
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	4	0.39
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	14	0.39
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	18	0.39
(1,480)	1:28:A:LYS:HB2	1:22:A:ARG:H	18	0.39
(1,477)	1:28:A:LYS:HB2	1:28:A:LYS:HE3	20	0.39
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	19	0.39
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	10	0.39
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	17	0.39
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	12	0.39
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	14	0.39
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	20	0.39
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	6	0.39
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	11	0.39
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	7	0.39
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	4	0.39
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	12	0.39
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	2	0.39
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	16	0.39
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	15	0.39
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	3	0.39
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	16	0.39
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	8	0.39
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	14	0.39
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	15	0.39
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	5	0.39
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	14	0.39
(1,142)	1:6:A:ASN:HA	1:7:A:PRO:HG2	4	0.39
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	17	0.39
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	8	0.39
(1,117)	1:5:A:PRO:HB2	1:5:A:PRO:HD2	1	0.39
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	3	0.39
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	16	0.39
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	17	0.39
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	20	0.39
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	16	0.39
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	18	0.39
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG21	15	0.39
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	15	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	5	0.38
(1,1886)	1:22:A:ARG:H	1:27:A:TYR:HD1	7	0.38
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	20	0.38
(1,1869)	1:53:A:GLY:H	1:51:A:LEU:HD22	5	0.38
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	3	0.38
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	12	0.38
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	19	0.38
(1,1756)	1:59:A:VAL:H	1:66:A:LYS:H	9	0.38
(1,1740)	1:57:A:GLY:H	1:66:A:LYS:HB2	6	0.38
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	12	0.38
(1,1602)	1:29:A:CYS:H	1:28:A:LYS:HD2	5	0.38
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	2	0.38
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	14	0.38
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	9	0.38
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	12	0.38
(1,1376)	1:82:A:LYS:H	1:82:A:LYS:HD2	9	0.38
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	2	0.38
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	5	0.38
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	2	0.38
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	9	0.38
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	15	0.38
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	3	0.38
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	6	0.38
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	15	0.38
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	2	0.38
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	5	0.38
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	16	0.38
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	17	0.38
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	19	0.38
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD12	14	0.38
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	9	0.38
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	4	0.38
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	11	0.38
(1,1193)	1:73:A:TYR:HB3	1:73:A:TYR:HD1	12	0.38
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	15	0.38
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	13	0.38
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	6	0.38
(1,1156)	1:69:A:CYS:HA	1:70:A:PRO:HG2	6	0.38
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	2	0.38
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	15	0.38
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	19	0.38
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	12	0.38
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	18	0.38
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	19	0.38
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	20	0.38
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	14	0.38
(1,1047)	1:58:A:TYR:H	1:65:A:TYR:HA	6	0.38
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	1	0.38
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	2	0.38
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	6	0.38
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	9	0.38
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	14	0.38
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	12	0.38
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	13	0.38
(1,872)	1:55:A:THR:HG23	1:67:A:CYS:HA	16	0.38
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	5	0.38
(1,837)	1:28:A:LYS:HB3	1:22:A:ARG:HD2	13	0.38
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	8	0.38
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	16	0.38
(1,822)	1:51:A:LEU:HD21	1:56:A:CYS:HB3	10	0.38
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	1	0.38
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	8	0.38
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	14	0.38
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	16	0.38
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	18	0.38
(1,707)	1:44:A:ALA:HB3	1:58:A:TYR:HD1	1	0.38
(1,703)	1:44:A:ALA:HB3	1:58:A:TYR:HA	14	0.38
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	5	0.38
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	5	0.38
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	8	0.38
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	2	0.38
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	5	0.38
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	20	0.38
(1,664)	1:40:A:CYS:HB2	1:31:A:CYS:HA	13	0.38
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	10	0.38
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	5	0.38
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG22	1	0.38
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	11	0.38
(1,549)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	12	0.38
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	20	0.38
(1,535)	1:32:A:ARG:HG2	1:40:A:CYS:HB2	8	0.38
(1,516)	1:32:A:ARG:HA	1:35:A:TYR:HD1	4	0.38
(1,381)	1:22:A:ARG:HB2	1:22:A:ARG:HD2	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	3	0.38
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	15	0.38
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	16	0.38
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	2	0.38
(1,304)	1:18:A:THR:HG21	1:30:A:TYR:HB2	9	0.38
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	20	0.38
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	6	0.38
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	1	0.38
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	9	0.38
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	16	0.38
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	16	0.38
(1,212)	1:10:A:PRO:HA	1:9:A:SER:H	9	0.38
(1,175)	1:8:A:CYS:H	1:7:A:PRO:HD2	17	0.38
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	13	0.38
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	4	0.38
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	17	0.38
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	3	0.38
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	10	0.38
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	17	0.38
(1,117)	1:5:A:PRO:HB2	1:5:A:PRO:HD2	10	0.38
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	19	0.38
(1,10)	1:31:A:CYS:HB2	1:32:A:ARG:HA	7	0.38
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	16	0.37
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	9	0.37
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	14	0.37
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	2	0.37
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	20	0.37
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	4	0.37
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	11	0.37
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	3	0.37
(1,1676)	1:79:A:GLN:H	1:75:A:GLY:HA2	8	0.37
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	2	0.37
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	20	0.37
(1,1620)	1:31:A:CYS:H	1:18:A:THR:HB	4	0.37
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	9	0.37
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	9	0.37
(1,1572)	1:23:A:GLY:H	1:22:A:ARG:HB2	6	0.37
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	17	0.37
(1,1527)	1:14:A:ARG:H	1:39:A:ASN:HA	13	0.37
(1,1510)	1:6:A:ASN:H	1:5:A:PRO:HB2	12	0.37
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	4	0.37
(1,1486)	1:7:A:PRO:HD3	1:6:A:ASN:HB3	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	12	0.37
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	6	0.37
(1,1436)	1:44:A:ALA:HB3	1:58:A:TYR:HE1	14	0.37
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	17	0.37
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	9	0.37
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	13	0.37
(1,1337)	1:81:A:LYS:HB2	1:83:A:TYR:HE1	10	0.37
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	16	0.37
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	2	0.37
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	12	0.37
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	16	0.37
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	20	0.37
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	1	0.37
(1,1191)	1:73:A:TYR:HB3	1:70:A:PRO:HD3	8	0.37
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	12	0.37
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	17	0.37
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	10	0.37
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	9	0.37
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	15	0.37
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	13	0.37
(1,1076)	1:67:A:CYS:HA	1:68:A:SER:HA	17	0.37
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	13	0.37
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	9	0.37
(1,1056)	1:66:A:LYS:H	1:65:A:TYR:HB2	18	0.37
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	16	0.37
(1,1047)	1:58:A:TYR:H	1:65:A:TYR:HA	9	0.37
(1,1036)	1:59:A:VAL:HG12	1:65:A:TYR:HA	17	0.37
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	3	0.37
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	7	0.37
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	12	0.37
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	4	0.37
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	18	0.37
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	19	0.37
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG12	3	0.37
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	18	0.37
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	2	0.37
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	9	0.37
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	14	0.37
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	11	0.37
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	4	0.37
(1,849)	1:54:A:GLY:HA2	1:70:A:PRO:HD2	7	0.37
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	9	0.37
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	11	0.37
(1,802)	1:50:A:CYS:H	1:50:A:CYS:HB2	8	0.37
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	2	0.37
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	3	0.37
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	4	0.37
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	12	0.37
(1,707)	1:44:A:ALA:HB2	1:58:A:TYR:HD1	6	0.37
(1,705)	1:44:A:ALA:HB2	1:65:A:TYR:HA	3	0.37
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	3	0.37
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	4	0.37
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	6	0.37
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	8	0.37
(1,666)	1:40:A:CYS:HB2	1:39:A:ASN:HA	2	0.37
(1,666)	1:40:A:CYS:HB2	1:39:A:ASN:HA	5	0.37
(1,666)	1:40:A:CYS:HB2	1:39:A:ASN:HA	18	0.37
(1,645)	1:39:A:ASN:HB3	1:41:A:GLN:HB3	6	0.37
(1,636)	1:38:A:LYS:HG3	1:38:A:LYS:HA	11	0.37
(1,551)	1:33:A:LYS:HB3	1:33:A:LYS:HE2	13	0.37
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	16	0.37
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	12	0.37
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	8	0.37
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	20	0.37
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	11	0.37
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	9	0.37
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	3	0.37
(1,408)	1:23:A:GLY:HA2	1:26:A:SER:H	10	0.37
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	5	0.37
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	11	0.37
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG22	14	0.37
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	4	0.37
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	9	0.37
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	10	0.37
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	16	0.37
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	9	0.37
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	8	0.37
(1,212)	1:10:A:PRO:HA	1:9:A:SER:H	6	0.37
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	19	0.37
(1,120)	1:5:A:PRO:HB3	1:5:A:PRO:HD3	16	0.37
(1,112)	1:5:A:PRO:HA	1:6:A:ASN:HA	6	0.37
(1,83)	1:2:A:VAL:HG22	1:4:A:TYR:HE1	9	0.37
(1,61)	1:71:A:TYR:HE1	1:71:A:TYR:HA	14	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	18	0.37
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	12	0.37
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	2	0.36
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	15	0.36
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	15	0.36
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	4	0.36
(1,1829)	1:76:A:LYS:H	1:76:A:LYS:HG3	1	0.36
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	12	0.36
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	16	0.36
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	5	0.36
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	17	0.36
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	1	0.36
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	11	0.36
(1,1703)	1:45:A:CYS:H	1:58:A:TYR:HD1	15	0.36
(1,1671)	1:41:A:GLN:H	1:39:A:ASN:HB3	18	0.36
(1,1658)	1:39:A:ASN:H	1:41:A:GLN:H	16	0.36
(1,1602)	1:29:A:CYS:H	1:28:A:LYS:HD2	8	0.36
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	4	0.36
(1,1500)	1:51:A:LEU:HD23	1:50:A:CYS:H	9	0.36
(1,1486)	1:7:A:PRO:HD3	1:6:A:ASN:HB3	13	0.36
(1,1436)	1:44:A:ALA:HB3	1:58:A:TYR:HE1	12	0.36
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	12	0.36
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	20	0.36
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	20	0.36
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	9	0.36
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	17	0.36
(1,1232)	1:76:A:LYS:HA	1:77:A:GLN:HA	7	0.36
(1,1223)	1:78:A:CYS:HA	1:77:A:GLN:HB2	17	0.36
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	19	0.36
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	2	0.36
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	18	0.36
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	14	0.36
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	10	0.36
(1,1131)	1:70:A:PRO:HB3	1:73:A:TYR:HD1	6	0.36
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	7	0.36
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	1	0.36
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	7	0.36
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	11	0.36
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	7	0.36
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	11	0.36
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	13	0.36
(1,988)	1:62:A:TYR:HA	1:62:A:TYR:HD1	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	5	0.36
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG11	5	0.36
(1,946)	1:59:A:VAL:HG13	1:61:A:GLY:HA3	20	0.36
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	6	0.36
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	13	0.36
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	20	0.36
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	12	0.36
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	10	0.36
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	14	0.36
(1,824)	1:51:A:LEU:HD23	1:51:A:LEU:H	15	0.36
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	11	0.36
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	1	0.36
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	19	0.36
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	6	0.36
(1,705)	1:44:A:ALA:HB3	1:65:A:TYR:HA	1	0.36
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	1	0.36
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	7	0.36
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	12	0.36
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	13	0.36
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	14	0.36
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	15	0.36
(1,636)	1:38:A:LYS:HG3	1:38:A:LYS:HA	6	0.36
(1,636)	1:38:A:LYS:HG3	1:38:A:LYS:HA	10	0.36
(1,629)	1:38:A:LYS:H	1:38:A:LYS:HB2	13	0.36
(1,603)	1:36:A:THR:HG22	1:42:A:TYR:HA	2	0.36
(1,600)	1:36:A:THR:HG21	1:64:A:TYR:HB2	5	0.36
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	11	0.36
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG21	7	0.36
(1,572)	1:35:A:TYR:HA	1:36:A:THR:HG21	8	0.36
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	15	0.36
(1,549)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	8	0.36
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	17	0.36
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	17	0.36
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	8	0.36
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	17	0.36
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	20	0.36
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	13	0.36
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	16	0.36
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD13	10	0.36
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	1	0.36
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	10	0.36
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	18	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	1	0.36
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	10	0.36
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	13	0.36
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	14	0.36
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	1	0.36
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	9	0.36
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	8	0.36
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	9	0.36
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	20	0.36
(1,176)	1:7:A:PRO:HG2	1:21:A:LYS:HG3	7	0.36
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	15	0.36
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	4	0.36
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	7	0.36
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	17	0.36
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	18	0.36
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	1	0.36
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	8	0.36
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	9	0.36
(1,12)	1:34:A:GLY:HA3	1:58:A:TYR:HB3	3	0.36
(1,6)	1:7:A:PRO:HD2	1:21:A:LYS:HE3	1	0.36
(1,1883)	1:67:A:CYS:H	1:65:A:TYR:HE1	6	0.35
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	12	0.35
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	8	0.35
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	4	0.35
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	9	0.35
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	11	0.35
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	16	0.35
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	5	0.35
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	8	0.35
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	20	0.35
(1,1808)	1:73:A:TYR:H	1:73:A:TYR:HB3	15	0.35
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	4	0.35
(1,1762)	1:61:A:GLY:H	1:60:A:TYR:HB2	14	0.35
(1,1703)	1:45:A:CYS:H	1:58:A:TYR:HD1	16	0.35
(1,1684)	1:42:A:TYR:H	1:39:A:ASN:HB2	6	0.35
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	1	0.35
(1,1625)	1:32:A:ARG:H	1:35:A:TYR:HB2	7	0.35
(1,1620)	1:31:A:CYS:H	1:18:A:THR:HB	8	0.35
(1,1603)	1:29:A:CYS:H	1:28:A:LYS:HE3	3	0.35
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	8	0.35
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	20	0.35
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1540)	1:17:A:GLY:H	1:13:A:CYS:HB2	17	0.35
(1,1515)	1:8:A:CYS:H	1:7:A:PRO:HG2	13	0.35
(1,1510)	1:6:A:ASN:H	1:5:A:PRO:HB2	8	0.35
(1,1500)	1:51:A:LEU:HD22	1:50:A:CYS:H	10	0.35
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	7	0.35
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	14	0.35
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	9	0.35
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	15	0.35
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	20	0.35
(1,1436)	1:44:A:ALA:HB1	1:58:A:TYR:HE1	7	0.35
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	3	0.35
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	15	0.35
(1,1379)	1:82:A:LYS:HE2	1:74:A:TYR:HE1	7	0.35
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	14	0.35
(1,1331)	1:81:A:LYS:HB2	1:81:A:LYS:HE2	20	0.35
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD11	15	0.35
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	18	0.35
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	2	0.35
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	5	0.35
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	19	0.35
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	6	0.35
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	1	0.35
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	16	0.35
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	12	0.35
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	20	0.35
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	20	0.35
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	12	0.35
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	17	0.35
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	20	0.35
(1,1056)	1:66:A:LYS:H	1:65:A:TYR:HB2	12	0.35
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	20	0.35
(1,1036)	1:59:A:VAL:HG12	1:65:A:TYR:HA	18	0.35
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	8	0.35
(1,955)	1:61:A:GLY:H	1:59:A:VAL:HG13	9	0.35
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG12	17	0.35
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG11	5	0.35
(1,872)	1:55:A:THR:HG22	1:67:A:CYS:HA	15	0.35
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	11	0.35
(1,849)	1:54:A:GLY:HA2	1:70:A:PRO:HD2	11	0.35
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	6	0.35
(1,824)	1:51:A:LEU:HD21	1:51:A:LEU:H	1	0.35
(1,824)	1:51:A:LEU:HD21	1:51:A:LEU:H	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,802)	1:50:A:CYS:H	1:50:A:CYS:HB2	4	0.35
(1,802)	1:50:A:CYS:H	1:50:A:CYS:HB2	10	0.35
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	6	0.35
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	15	0.35
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	9	0.35
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	16	0.35
(1,599)	1:36:A:THR:HG22	1:64:A:TYR:HB3	7	0.35
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	3	0.35
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	4	0.35
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	13	0.35
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	7	0.35
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	19	0.35
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	15	0.35
(1,405)	1:23:A:GLY:HA2	1:22:A:ARG:HA	13	0.35
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	4	0.35
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	7	0.35
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	9	0.35
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	17	0.35
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	12	0.35
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	18	0.35
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	19	0.35
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	7	0.35
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	13	0.35
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	2	0.35
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	20	0.35
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	13	0.35
(1,117)	1:5:A:PRO:HB2	1:5:A:PRO:HD2	13	0.35
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	8	0.35
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	14	0.35
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	7	0.35
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	14	0.35
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	20	0.35
(1,38)	1:82:A:LYS:H	1:74:A:TYR:HE1	17	0.35
(1,9)	1:31:A:CYS:HB2	1:32:A:ARG:HB3	9	0.35
(1,8)	1:31:A:CYS:HB3	1:32:A:ARG:HG2	12	0.35
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE2	9	0.35
(1,1886)	1:22:A:ARG:H	1:27:A:TYR:HD1	14	0.34
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	7	0.34
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	9	0.34
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	5	0.34
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	20	0.34
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	17	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	11	0.34
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	1	0.34
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	4	0.34
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	6	0.34
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	9	0.34
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	11	0.34
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	15	0.34
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	19	0.34
(1,1754)	1:59:A:VAL:H	1:58:A:TYR:HD1	11	0.34
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	9	0.34
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	10	0.34
(1,1703)	1:45:A:CYS:H	1:58:A:TYR:HD1	18	0.34
(1,1676)	1:79:A:GLN:H	1:75:A:GLY:HA2	6	0.34
(1,1658)	1:39:A:ASN:H	1:41:A:GLN:H	3	0.34
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	17	0.34
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	13	0.34
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	14	0.34
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	6	0.34
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	6	0.34
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	6	0.34
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	11	0.34
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	17	0.34
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	18	0.34
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	7	0.34
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	16	0.34
(1,1436)	1:44:A:ALA:HB2	1:58:A:TYR:HE1	19	0.34
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	5	0.34
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	20	0.34
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	18	0.34
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	17	0.34
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	6	0.34
(1,1337)	1:81:A:LYS:HB2	1:83:A:TYR:HE1	2	0.34
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	20	0.34
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	19	0.34
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD12	18	0.34
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	13	0.34
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	17	0.34
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	5	0.34
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	10	0.34
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	16	0.34
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	19	0.34
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	10	0.34
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	2	0.34
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	16	0.34
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	16	0.34
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	1	0.34
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	5	0.34
(1,1036)	1:59:A:VAL:HG13	1:65:A:TYR:HA	8	0.34
(1,1036)	1:59:A:VAL:HG11	1:65:A:TYR:HA	16	0.34
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	16	0.34
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	17	0.34
(1,1015)	1:64:A:TYR:H	1:63:A:PRO:HG3	15	0.34
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	12	0.34
(1,970)	1:60:A:TYR:HA	1:60:A:TYR:HD1	20	0.34
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG13	7	0.34
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	2	0.34
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	8	0.34
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	19	0.34
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	15	0.34
(1,872)	1:55:A:THR:HG23	1:67:A:CYS:HA	20	0.34
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	8	0.34
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	16	0.34
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	17	0.34
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	19	0.34
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	1	0.34
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	4	0.34
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	19	0.34
(1,824)	1:51:A:LEU:HD21	1:51:A:LEU:H	18	0.34
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	13	0.34
(1,802)	1:50:A:CYS:H	1:50:A:CYS:HB2	14	0.34
(1,802)	1:50:A:CYS:H	1:50:A:CYS:HB2	15	0.34
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	4	0.34
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	14	0.34
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	10	0.34
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	17	0.34
(1,707)	1:44:A:ALA:HB3	1:58:A:TYR:HD1	9	0.34
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	1	0.34
(1,648)	1:39:A:ASN:HB2	1:41:A:GLN:HB2	19	0.34
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	16	0.34
(1,592)	1:36:A:THR:HB	1:44:A:ALA:HB2	5	0.34
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	18	0.34
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	7	0.34
(1,526)	1:33:A:LYS:H	1:32:A:ARG:HB2	16	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	20	0.34
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	4	0.34
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	14	0.34
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	16	0.34
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	9	0.34
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	20	0.34
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	9	0.34
(1,387)	1:22:A:ARG:HA	1:22:A:ARG:HD2	17	0.34
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	7	0.34
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	10	0.34
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	11	0.34
(1,307)	1:18:A:THR:HG23	1:30:A:TYR:HE1	20	0.34
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	17	0.34
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	16	0.34
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	15	0.34
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	18	0.34
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	11	0.34
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	11	0.34
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	6	0.34
(1,249)	1:13:A:CYS:HB2	1:11:A:TYR:HD1	20	0.34
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	11	0.34
(1,206)	1:9:A:SER:H	1:9:A:SER:HB2	19	0.34
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	2	0.34
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	3	0.34
(1,117)	1:5:A:PRO:HB2	1:5:A:PRO:HD2	17	0.34
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	1	0.34
(1,100)	1:4:A:TYR:HB2	1:2:A:VAL:HG22	9	0.34
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	8	0.34
(1,96)	1:3:A:TYR:HB2	1:3:A:TYR:H	14	0.34
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	1	0.34
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	6	0.34
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	8	0.34
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	11	0.34
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	13	0.34
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	15	0.34
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	19	0.34
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	9	0.34
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	8	0.34
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	20	0.34
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	16	0.34
(1,13)	1:34:A:GLY:HA2	1:58:A:TYR:HB3	10	0.34
(1,12)	1:34:A:GLY:HA3	1:58:A:TYR:HB3	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	20	0.33
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	15	0.33
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	18	0.33
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	9	0.33
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	8	0.33
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	13	0.33
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	18	0.33
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	18	0.33
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	2	0.33
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	3	0.33
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	16	0.33
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	17	0.33
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	18	0.33
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	20	0.33
(1,1759)	1:61:A:GLY:H	1:59:A:VAL:HB	2	0.33
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	12	0.33
(1,1636)	1:34:A:GLY:H	1:35:A:TYR:HD1	3	0.33
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	18	0.33
(1,1572)	1:23:A:GLY:H	1:22:A:ARG:HB2	11	0.33
(1,1568)	1:21:A:LYS:H	1:27:A:TYR:HB2	11	0.33
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	9	0.33
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	20	0.33
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	20	0.33
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	7	0.33
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	20	0.33
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	3	0.33
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	5	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	1	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	4	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	6	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	8	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	9	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	10	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	11	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	13	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	14	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	15	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	17	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	18	0.33
(1,1443)	1:38:A:LYS:HD2	1:38:A:LYS:HE2	20	0.33
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	3	0.33
(1,1420)	1:58:A:TYR:HA	1:66:A:LYS:HA	14	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	7	0.33
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	8	0.33
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	15	0.33
(1,1353)	1:82:A:LYS:HA	1:74:A:TYR:HD1	2	0.33
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	2	0.33
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	8	0.33
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	10	0.33
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	11	0.33
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	14	0.33
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	20	0.33
(1,1347)	1:82:A:LYS:HA	1:82:A:LYS:HG2	13	0.33
(1,1337)	1:81:A:LYS:HB2	1:83:A:TYR:HE1	1	0.33
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	3	0.33
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	5	0.33
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	20	0.33
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	18	0.33
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD12	8	0.33
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	6	0.33
(1,1201)	1:74:A:TYR:HB3	1:75:A:GLY:H	15	0.33
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	4	0.33
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	6	0.33
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	8	0.33
(1,1191)	1:73:A:TYR:HB3	1:70:A:PRO:HD3	17	0.33
(1,1182)	1:72:A:GLY:HA2	1:71:A:TYR:HD1	4	0.33
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	1	0.33
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	7	0.33
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	9	0.33
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	18	0.33
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	2	0.33
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	9	0.33
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	1	0.33
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	18	0.33
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	8	0.33
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	9	0.33
(1,1015)	1:64:A:TYR:H	1:63:A:PRO:HG3	8	0.33
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	9	0.33
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	15	0.33
(1,938)	1:59:A:VAL:HG11	1:59:A:VAL:HG22	4	0.33
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG22	19	0.33
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	3	0.33
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	7	0.33
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	16	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	3	0.33
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	2	0.33
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	17	0.33
(1,804)	1:51:A:LEU:H	1:50:A:CYS:HB3	11	0.33
(1,802)	1:50:A:CYS:H	1:50:A:CYS:HB2	16	0.33
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	20	0.33
(1,798)	1:50:A:CYS:HA	1:77:A:GLN:HA	9	0.33
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	5	0.33
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	19	0.33
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	11	0.33
(1,705)	1:44:A:ALA:HB3	1:65:A:TYR:HA	5	0.33
(1,705)	1:44:A:ALA:HB2	1:65:A:TYR:HA	15	0.33
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	12	0.33
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	18	0.33
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	6	0.33
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	8	0.33
(1,597)	1:36:A:THR:HG22	1:42:A:TYR:HB3	5	0.33
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	10	0.33
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	1	0.33
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	3	0.33
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	5	0.33
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	5	0.33
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	4	0.33
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	7	0.33
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	12	0.33
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	13	0.33
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	14	0.33
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	16	0.33
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	18	0.33
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	19	0.33
(1,391)	1:22:A:ARG:HG3	1:27:A:TYR:HA	7	0.33
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	19	0.33
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	16	0.33
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	8	0.33
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	18	0.33
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG21	16	0.33
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	6	0.33
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	16	0.33
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	9	0.33
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	5	0.33
(1,206)	1:9:A:SER:H	1:9:A:SER:HB2	16	0.33
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	13	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	20	0.33
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	10	0.33
(1,150)	1:6:A:ASN:HA	1:21:A:LYS:HG3	6	0.33
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	6	0.33
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	1	0.33
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	4	0.33
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	5	0.33
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	6	0.33
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	10	0.33
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	13	0.33
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	4	0.33
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	9	0.33
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	16	0.33
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	17	0.33
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	17	0.33
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	15	0.33
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	4	0.33
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	18	0.33
(1,12)	1:34:A:GLY:HA3	1:58:A:TYR:HB3	5	0.33
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	14	0.32
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	1	0.32
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	2	0.32
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	7	0.32
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	9	0.32
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	15	0.32
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	15	0.32
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	16	0.32
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	7	0.32
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	10	0.32
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	3	0.32
(1,1754)	1:59:A:VAL:H	1:58:A:TYR:HD1	13	0.32
(1,1709)	1:46:A:PHE:H	1:46:A:PHE:HD1	18	0.32
(1,1698)	1:44:A:ALA:H	1:58:A:TYR:HE1	6	0.32
(1,1676)	1:79:A:GLN:H	1:75:A:GLY:HA2	12	0.32
(1,1637)	1:35:A:TYR:H	1:32:A:ARG:HB3	3	0.32
(1,1539)	1:17:A:GLY:H	1:32:A:ARG:HG2	4	0.32
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	6	0.32
(1,1510)	1:6:A:ASN:H	1:5:A:PRO:HB2	9	0.32
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	7	0.32
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	11	0.32
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	16	0.32
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	19	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	2	0.32
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	14	0.32
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	5	0.32
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	12	0.32
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	19	0.32
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	16	0.32
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	10	0.32
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	4	0.32
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	1	0.32
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	3	0.32
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	4	0.32
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	7	0.32
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	9	0.32
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	12	0.32
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	13	0.32
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	15	0.32
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	16	0.32
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	17	0.32
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	19	0.32
(1,1347)	1:82:A:LYS:HA	1:82:A:LYS:HG2	1	0.32
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	12	0.32
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	18	0.32
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	1	0.32
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	8	0.32
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	11	0.32
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	11	0.32
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	9	0.32
(1,1151)	1:69:A:CYS:H	1:70:A:PRO:HD2	3	0.32
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	3	0.32
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	18	0.32
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	20	0.32
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	11	0.32
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	14	0.32
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	19	0.32
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	12	0.32
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	18	0.32
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	9	0.32
(1,1036)	1:59:A:VAL:HG12	1:65:A:TYR:HA	5	0.32
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	5	0.32
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	19	0.32
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	7	0.32
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG13	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG23	1	0.32
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	10	0.32
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	18	0.32
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	7	0.32
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	8	0.32
(1,865)	1:55:A:THR:HG21	1:56:A:CYS:HB3	6	0.32
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	14	0.32
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	18	0.32
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	20	0.32
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	6	0.32
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	13	0.32
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	20	0.32
(1,804)	1:51:A:LEU:H	1:50:A:CYS:HB3	14	0.32
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	6	0.32
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	14	0.32
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	3	0.32
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	9	0.32
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	17	0.32
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	20	0.32
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	1	0.32
(1,734)	1:46:A:PHE:HB3	1:46:A:PHE:HD1	17	0.32
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	12	0.32
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	14	0.32
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	7	0.32
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	9	0.32
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	18	0.32
(1,519)	1:32:A:ARG:HB3	1:32:A:ARG:HD2	9	0.32
(1,489)	1:29:A:CYS:HA	1:18:A:THR:HG22	11	0.32
(1,480)	1:28:A:LYS:HB2	1:22:A:ARG:H	6	0.32
(1,480)	1:28:A:LYS:HB2	1:22:A:ARG:H	15	0.32
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	13	0.32
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	6	0.32
(1,434)	1:26:A:SER:H	1:25:A:TYR:HB3	15	0.32
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	4	0.32
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	5	0.32
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	10	0.32
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	17	0.32
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	20	0.32
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	10	0.32
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	15	0.32
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	7	0.32
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	11	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	19	0.32
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	18	0.32
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	17	0.32
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	1	0.32
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	4	0.32
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	8	0.32
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	12	0.32
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	18	0.32
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	5	0.32
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	19	0.32
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	20	0.32
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	10	0.32
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	17	0.32
(1,12)	1:34:A:GLY:HA3	1:58:A:TYR:HB3	4	0.32
(1,6)	1:7:A:PRO:HD2	1:21:A:LYS:HE3	5	0.32
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	6	0.31
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	19	0.31
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	6	0.31
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	11	0.31
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	10	0.31
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	3	0.31
(1,1776)	1:65:A:TYR:H	1:59:A:VAL:HB	20	0.31
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	10	0.31
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	2	0.31
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	13	0.31
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	18	0.31
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	4	0.31
(1,1603)	1:29:A:CYS:H	1:28:A:LYS:HE3	11	0.31
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	16	0.31
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	18	0.31
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	18	0.31
(1,1500)	1:51:A:LEU:HD21	1:50:A:CYS:H	17	0.31
(1,1494)	1:2:A:VAL:HG13	1:4:A:TYR:HE1	13	0.31
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	3	0.31
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	15	0.31
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	1	0.31
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	15	0.31
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	3	0.31
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	9	0.31
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	2	0.31
(1,1398)	1:78:A:CYS:HA	1:69:A:CYS:HB3	6	0.31
(1,1375)	1:83:A:TYR:H	1:82:A:LYS:HD2	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	5	0.31
(1,1348)	1:82:A:LYS:HA	1:82:A:LYS:HB3	18	0.31
(1,1347)	1:82:A:LYS:HA	1:82:A:LYS:HG2	19	0.31
(1,1300)	1:79:A:GLN:HG3	1:80:A:LEU:HB2	9	0.31
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	13	0.31
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	12	0.31
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD12	5	0.31
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD12	9	0.31
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	4	0.31
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	4	0.31
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	14	0.31
(1,1181)	1:72:A:GLY:HA2	1:73:A:TYR:HD1	2	0.31
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	19	0.31
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	18	0.31
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	2	0.31
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	16	0.31
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	6	0.31
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	13	0.31
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	17	0.31
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	14	0.31
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG13	20	0.31
(1,958)	1:66:A:LYS:H	1:59:A:VAL:HG12	6	0.31
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG13	1	0.31
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG12	13	0.31
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG22	9	0.31
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG22	12	0.31
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	2	0.31
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	19	0.31
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	2	0.31
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	9	0.31
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	13	0.31
(1,840)	1:53:A:GLY:HA2	1:70:A:PRO:HG2	6	0.31
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	7	0.31
(1,824)	1:51:A:LEU:HD21	1:51:A:LEU:H	6	0.31
(1,824)	1:51:A:LEU:HD23	1:51:A:LEU:H	8	0.31
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	16	0.31
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	7	0.31
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	16	0.31
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	3	0.31
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	11	0.31
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	6	0.31
(1,688)	1:44:A:ALA:HA	1:36:A:THR:HG22	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,688)	1:44:A:ALA:HA	1:36:A:THR:HG22	15	0.31
(1,605)	1:37:A:GLY:H	1:36:A:THR:HG22	7	0.31
(1,600)	1:36:A:THR:HG23	1:64:A:TYR:HB2	6	0.31
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	2	0.31
(1,569)	1:34:A:GLY:HA2	1:58:A:TYR:HD1	17	0.31
(1,549)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	13	0.31
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	6	0.31
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	3	0.31
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	1	0.31
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	3	0.31
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	11	0.31
(1,380)	1:22:A:ARG:HB2	1:22:A:ARG:HG2	3	0.31
(1,380)	1:22:A:ARG:HB2	1:22:A:ARG:HG2	5	0.31
(1,380)	1:22:A:ARG:HB2	1:22:A:ARG:HG2	6	0.31
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	12	0.31
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	12	0.31
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	7	0.31
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	5	0.31
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	12	0.31
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	14	0.31
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	15	0.31
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	17	0.31
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	18	0.31
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	20	0.31
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	5	0.31
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	9	0.31
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	9	0.31
(1,128)	1:5:A:PRO:HD2	1:4:A:TYR:HA	12	0.31
(1,98)	1:4:A:TYR:HA	1:4:A:TYR:HD1	14	0.31
(1,96)	1:3:A:TYR:HB2	1:3:A:TYR:H	18	0.31
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	2	0.31
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	3	0.31
(1,58)	1:71:A:TYR:H	1:71:A:TYR:HD1	8	0.31
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	8	0.31
(1,38)	1:82:A:LYS:H	1:74:A:TYR:HE1	18	0.31
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	1	0.31
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	19	0.31
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	5	0.31
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	15	0.31
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	20	0.31
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	15	0.3
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	13	0.3
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	18	0.3
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	1	0.3
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	14	0.3
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	13	0.3
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	17	0.3
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	18	0.3
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	8	0.3
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	14	0.3
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	11	0.3
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	13	0.3
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	20	0.3
(1,1666)	1:79:A:GLN:H	1:80:A:LEU:HD12	12	0.3
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	14	0.3
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	16	0.3
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	5	0.3
(1,1607)	1:30:A:TYR:H	1:20:A:LYS:HB3	13	0.3
(1,1603)	1:29:A:CYS:H	1:28:A:LYS:HE3	15	0.3
(1,1602)	1:29:A:CYS:H	1:28:A:LYS:HD2	6	0.3
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	11	0.3
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	14	0.3
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	20	0.3
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	15	0.3
(1,1477)	1:18:A:THR:HG21	1:19:A:CYS:HB3	5	0.3
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	15	0.3
(1,1410)	1:70:A:PRO:HG2	1:54:A:GLY:H	3	0.3
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	1	0.3
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	13	0.3
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	4	0.3
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	6	0.3
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	13	0.3
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	15	0.3
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	11	0.3
(1,1242)	1:77:A:GLN:HG3	1:49:A:PRO:HB3	4	0.3
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	2	0.3
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	16	0.3
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	13	0.3
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	3	0.3
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	5	0.3
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	10	0.3
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	2	0.3
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	17	0.3
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	8	0.3
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	2	0.3
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	7	0.3
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	8	0.3
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	12	0.3
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	20	0.3
(1,1036)	1:59:A:VAL:HG13	1:65:A:TYR:HA	3	0.3
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	2	0.3
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	1	0.3
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG12	19	0.3
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG13	8	0.3
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG13	20	0.3
(1,938)	1:59:A:VAL:HG13	1:59:A:VAL:HG22	18	0.3
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG21	20	0.3
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	4	0.3
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	9	0.3
(1,868)	1:55:A:THR:HG21	1:68:A:SER:HB2	6	0.3
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	10	0.3
(1,849)	1:54:A:GLY:HA2	1:70:A:PRO:HD2	1	0.3
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	8	0.3
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	1	0.3
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	7	0.3
(1,699)	1:44:A:ALA:HB1	1:64:A:TYR:HB3	12	0.3
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	4	0.3
(1,658)	1:40:A:CYS:HB3	1:31:A:CYS:HB3	20	0.3
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	9	0.3
(1,588)	1:58:A:TYR:HB2	1:59:A:VAL:H	8	0.3
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	2	0.3
(1,550)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	5	0.3
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	14	0.3
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	6	0.3
(1,444)	1:74:A:TYR:HA	1:74:A:TYR:HB2	15	0.3
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	6	0.3
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	2	0.3
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	13	0.3
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG22	11	0.3
(1,297)	1:18:A:THR:HB	1:30:A:TYR:HE1	13	0.3
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	6	0.3
(1,286)	1:18:A:THR:HA	1:30:A:TYR:HD1	16	0.3
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	19	0.3
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	17	0.3
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	16	0.3
(1,181)	1:7:A:PRO:HG2	1:27:A:TYR:HA	1	0.3
(1,150)	1:6:A:ASN:HA	1:21:A:LYS:HG3	7	0.3
(1,140)	1:70:A:PRO:HG3	1:54:A:GLY:H	12	0.3
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	19	0.3
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	1	0.3
(1,117)	1:5:A:PRO:HB2	1:5:A:PRO:HD2	2	0.3
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	3	0.3
(1,88)	1:3:A:TYR:HA	1:2:A:VAL:HA	10	0.3
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	3	0.3
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	19	0.3
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	12	0.3
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	13	0.3
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	14	0.3
(1,10)	1:31:A:CYS:HB2	1:32:A:ARG:HA	8	0.3
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	17	0.29
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	9	0.29
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	4	0.29
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	12	0.29
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	19	0.29
(1,1776)	1:65:A:TYR:H	1:59:A:VAL:HB	16	0.29
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	2	0.29
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	17	0.29
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	10	0.29
(1,1709)	1:46:A:PHE:H	1:46:A:PHE:HD1	12	0.29
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	1	0.29
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD21	1	0.29
(1,1572)	1:23:A:GLY:H	1:22:A:ARG:HB2	1	0.29
(1,1572)	1:23:A:GLY:H	1:22:A:ARG:HB2	8	0.29
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	15	0.29
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	13	0.29
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	14	0.29
(1,1514)	1:6:A:ASN:H	1:7:A:PRO:HD2	19	0.29
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	2	0.29
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	19	0.29
(1,1500)	1:51:A:LEU:HD21	1:50:A:CYS:H	4	0.29
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	8	0.29
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	7	0.29
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	10	0.29
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	2	0.29
(1,1436)	1:44:A:ALA:HB2	1:58:A:TYR:HE1	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	20	0.29
(1,1398)	1:78:A:CYS:HA	1:69:A:CYS:HB3	13	0.29
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	14	0.29
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	10	0.29
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	10	0.29
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	11	0.29
(1,1319)	1:79:A:GLN:HG3	1:80:A:LEU:HD23	13	0.29
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	12	0.29
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	15	0.29
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	10	0.29
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	5	0.29
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	11	0.29
(1,1200)	1:75:A:GLY:H	1:74:A:TYR:HB2	13	0.29
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	1	0.29
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	10	0.29
(1,1158)	1:70:A:PRO:HG2	1:73:A:TYR:H	4	0.29
(1,1133)	1:71:A:TYR:H	1:70:A:PRO:HB2	19	0.29
(1,1128)	1:69:A:CYS:HA	1:70:A:PRO:HB3	3	0.29
(1,1112)	1:70:A:PRO:HA	1:70:A:PRO:HG3	3	0.29
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	5	0.29
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	18	0.29
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	5	0.29
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	5	0.29
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	4	0.29
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	10	0.29
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	15	0.29
(1,1015)	1:64:A:TYR:H	1:63:A:PRO:HG3	18	0.29
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	16	0.29
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG13	2	0.29
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG12	5	0.29
(1,941)	1:66:A:LYS:HB2	1:59:A:VAL:HG13	3	0.29
(1,938)	1:59:A:VAL:HG11	1:59:A:VAL:HG23	8	0.29
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG23	16	0.29
(1,897)	1:57:A:GLY:HA2	1:58:A:TYR:HD1	3	0.29
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	4	0.29
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	11	0.29
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	15	0.29
(1,872)	1:55:A:THR:HG23	1:67:A:CYS:HA	11	0.29
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	7	0.29
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	16	0.29
(1,836)	1:52:A:ASN:HB3	1:78:A:CYS:HB3	11	0.29
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	13	0.29
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	16	0.29
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	8	0.29
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	9	0.29
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	18	0.29
(1,717)	1:45:A:CYS:HA	1:58:A:TYR:HE1	10	0.29
(1,707)	1:44:A:ALA:HB2	1:58:A:TYR:HD1	4	0.29
(1,688)	1:44:A:ALA:HA	1:36:A:THR:HG21	3	0.29
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	6	0.29
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	8	0.29
(1,684)	1:43:A:ASN:HA	1:46:A:PHE:H	17	0.29
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	17	0.29
(1,666)	1:40:A:CYS:HB2	1:39:A:ASN:HA	7	0.29
(1,655)	1:40:A:CYS:HA	1:39:A:ASN:H	7	0.29
(1,636)	1:38:A:LYS:HG3	1:38:A:LYS:HA	13	0.29
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	2	0.29
(1,603)	1:36:A:THR:HG22	1:42:A:TYR:HA	5	0.29
(1,573)	1:73:A:TYR:HA	1:81:A:LYS:HG2	2	0.29
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	3	0.29
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	16	0.29
(1,516)	1:32:A:ARG:HA	1:35:A:TYR:HD1	14	0.29
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	19	0.29
(1,473)	1:66:A:LYS:HB3	1:59:A:VAL:HG11	20	0.29
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	9	0.29
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	15	0.29
(1,450)	1:26:A:SER:HA	1:22:A:ARG:H	10	0.29
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	1	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	1	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	2	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	4	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	7	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	9	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	11	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	12	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	13	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	14	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	15	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	16	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	18	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	19	0.29
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	20	0.29
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	15	0.29
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	1	0.29
(1,337)	1:20:A:LYS:HD3	1:30:A:TYR:HD1	19	0.29
(1,307)	1:18:A:THR:HG21	1:30:A:TYR:HE1	19	0.29
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	20	0.29
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	5	0.29
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	1	0.29
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	14	0.29
(1,230)	1:10:A:PRO:HG3	1:11:A:TYR:H	11	0.29
(1,230)	1:10:A:PRO:HG3	1:11:A:TYR:H	13	0.29
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	1	0.29
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	5	0.29
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	2	0.29
(1,78)	1:21:A:LYS:HB2	1:27:A:TYR:HB2	15	0.29
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	7	0.29
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	16	0.29
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	19	0.29
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	4	0.29
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	10	0.29
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	1	0.28
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	18	0.28
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	20	0.28
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	18	0.28
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	2	0.28
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	7	0.28
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	9	0.28
(1,1855)	1:81:A:LYS:H	1:80:A:LEU:H	17	0.28
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	5	0.28
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	5	0.28
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	8	0.28
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	12	0.28
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	5	0.28
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	12	0.28
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	4	0.28
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	13	0.28
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	17	0.28
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	16	0.28
(1,1635)	1:34:A:GLY:H	1:33:A:LYS:HB3	7	0.28
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	7	0.28
(1,1619)	1:31:A:CYS:H	1:30:A:TYR:HB2	13	0.28
(1,1619)	1:31:A:CYS:H	1:30:A:TYR:HB2	18	0.28
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	14	0.28
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	6	0.28
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	16	0.28
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	20	0.28
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	12	0.28
(1,1477)	1:18:A:THR:HG21	1:19:A:CYS:HB3	1	0.28
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	8	0.28
(1,1426)	1:53:A:GLY:HA2	1:52:A:ASN:H	15	0.28
(1,1417)	1:63:A:PRO:HB2	1:64:A:TYR:HD1	7	0.28
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	5	0.28
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	8	0.28
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	19	0.28
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	20	0.28
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	1	0.28
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	19	0.28
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	3	0.28
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	20	0.28
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	16	0.28
(1,1362)	1:82:A:LYS:HB3	1:81:A:LYS:HA	6	0.28
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	8	0.28
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	5	0.28
(1,1317)	1:80:A:LEU:HD22	1:80:A:LEU:HD11	13	0.28
(1,1310)	1:79:A:GLN:HG2	1:80:A:LEU:HD12	7	0.28
(1,1178)	1:72:A:GLY:HA3	1:82:A:LYS:HB2	10	0.28
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	16	0.28
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	10	0.28
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	1	0.28
(1,1133)	1:71:A:TYR:H	1:70:A:PRO:HB2	16	0.28
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	1	0.28
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	5	0.28
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	15	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	1	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	2	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	3	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	4	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	5	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	6	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	7	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	9	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	10	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	12	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	14	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	17	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	18	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	19	0.28
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	20	0.28
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	19	0.28
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	1	0.28
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	2	0.28
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	12	0.28
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	6	0.28
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	13	0.28
(1,938)	1:59:A:VAL:HG11	1:59:A:VAL:HG22	7	0.28
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG23	11	0.28
(1,938)	1:59:A:VAL:HG11	1:59:A:VAL:HG21	15	0.28
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	18	0.28
(1,891)	1:57:A:GLY:HA2	1:66:A:LYS:HB2	2	0.28
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	1	0.28
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	4	0.28
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	6	0.28
(1,849)	1:54:A:GLY:HA2	1:70:A:PRO:HD2	17	0.28
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	8	0.28
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	12	0.28
(1,831)	1:51:A:LEU:HB2	1:52:A:ASN:HA	15	0.28
(1,822)	1:51:A:LEU:HD22	1:56:A:CYS:HB3	14	0.28
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	6	0.28
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	18	0.28
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	2	0.28
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	9	0.28
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	13	0.28
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	20	0.28
(1,705)	1:44:A:ALA:HB2	1:65:A:TYR:HA	13	0.28
(1,695)	1:44:A:ALA:HB3	1:45:A:CYS:HB3	12	0.28
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	15	0.28
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	10	0.28
(1,659)	1:40:A:CYS:HB2	1:35:A:TYR:HB3	4	0.28
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	8	0.28
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG21	20	0.28
(1,597)	1:36:A:THR:HG21	1:42:A:TYR:HB3	13	0.28
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	20	0.28
(1,565)	1:34:A:GLY:HA3	1:35:A:TYR:HD1	17	0.28
(1,557)	1:34:A:GLY:H	1:33:A:LYS:HE2	20	0.28
(1,550)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	9	0.28
(1,550)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	15	0.28
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	18	0.28
(1,532)	1:32:A:ARG:HD2	1:32:A:ARG:H	4	0.28
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	8	0.28
(1,455)	1:27:A:TYR:HA	1:21:A:LYS:HB2	15	0.28
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	6	0.28
(1,420)	1:25:A:TYR:H	1:24:A:LEU:HA	8	0.28
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	9	0.28
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	12	0.28
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	8	0.28
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	10	0.28
(1,394)	1:22:A:ARG:HB3	1:22:A:ARG:HG2	17	0.28
(1,393)	1:22:A:ARG:HG3	1:28:A:LYS:H	19	0.28
(1,370)	1:21:A:LYS:HG3	1:23:A:GLY:HA2	8	0.28
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	15	0.28
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG21	6	0.28
(1,297)	1:18:A:THR:HB	1:30:A:TYR:HE1	18	0.28
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	11	0.28
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	17	0.28
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	2	0.28
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	6	0.28
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	3	0.28
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	20	0.28
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	10	0.28
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	19	0.28
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	4	0.28
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	5	0.28
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	17	0.28
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	4	0.28
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	7	0.28
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	11	0.28
(1,171)	1:7:A:PRO:HD3	1:8:A:CYS:H	7	0.28
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	13	0.28
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	17	0.28
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	2	0.28
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	19	0.28
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	10	0.28
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	15	0.28
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	2	0.28
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	20	0.28
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	9	0.28
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	10	0.28
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	1	0.28
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	2	0.28
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	11	0.28
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	9	0.27
(1,1869)	1:53:A:GLY:H	1:51:A:LEU:HD23	19	0.27
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	1	0.27
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	10	0.27
(1,1776)	1:65:A:TYR:H	1:59:A:VAL:HB	13	0.27
(1,1696)	1:44:A:ALA:H	1:43:A:ASN:HB2	3	0.27
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	7	0.27
(1,1645)	1:35:A:TYR:H	1:33:A:LYS:HG2	7	0.27
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	10	0.27
(1,1619)	1:31:A:CYS:H	1:30:A:TYR:HB2	20	0.27
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	18	0.27
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	7	0.27
(1,1572)	1:23:A:GLY:H	1:22:A:ARG:HB2	5	0.27
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	19	0.27
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	11	0.27
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	19	0.27
(1,1523)	1:14:A:ARG:H	1:14:A:ARG:HG2	13	0.27
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	13	0.27
(1,1485)	1:10:A:PRO:HB3	1:11:A:TYR:HB2	1	0.27
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	5	0.27
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	13	0.27
(1,1457)	1:32:A:ARG:H	1:32:A:ARG:HG2	9	0.27
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	7	0.27
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	7	0.27
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	7	0.27
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	9	0.27
(1,1395)	1:80:A:LEU:HA	1:81:A:LYS:HB2	4	0.27
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	11	0.27
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	2	0.27
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD11	4	0.27
(1,1317)	1:80:A:LEU:HD21	1:80:A:LEU:HD13	5	0.27
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD13	6	0.27
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD13	10	0.27
(1,1317)	1:80:A:LEU:HD22	1:80:A:LEU:HD12	20	0.27
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	5	0.27
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	15	0.27
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD13	15	0.27
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	7	0.27
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	10	0.27
(1,1142)	1:54:A:GLY:HA3	1:70:A:PRO:HD2	3	0.27
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	8	0.27
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	11	0.27
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	15	0.27
(1,1083)	1:68:A:SER:HB2	1:68:A:SER:HA	16	0.27
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	4	0.27
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	10	0.27
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	19	0.27
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG13	5	0.27
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG11	7	0.27
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	6	0.27
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	18	0.27
(1,1029)	1:64:A:TYR:HB2	1:63:A:PRO:HB3	11	0.27
(1,988)	1:62:A:TYR:HA	1:62:A:TYR:HD1	7	0.27
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	20	0.27
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG13	16	0.27
(1,940)	1:59:A:VAL:HG12	1:66:A:LYS:HG2	11	0.27
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG21	2	0.27
(1,938)	1:59:A:VAL:HG13	1:59:A:VAL:HG21	6	0.27
(1,924)	1:59:A:VAL:HA	1:58:A:TYR:HB3	16	0.27
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	7	0.27
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	17	0.27
(1,869)	1:55:A:THR:HG23	1:68:A:SER:HB3	12	0.27
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	4	0.27
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	4	0.27
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	6	0.27
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	7	0.27
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	9	0.27
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	10	0.27
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	5	0.27
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	8	0.27
(1,751)	1:47:A:PRO:HD3	1:47:A:PRO:HG2	11	0.27
(1,751)	1:47:A:PRO:HD3	1:47:A:PRO:HG2	18	0.27
(1,724)	1:45:A:CYS:HB3	1:58:A:TYR:HD1	14	0.27
(1,699)	1:44:A:ALA:HB3	1:64:A:TYR:HB3	18	0.27
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	1	0.27
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	3	0.27
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	10	0.27
(1,648)	1:39:A:ASN:HB2	1:41:A:GLN:HB2	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:37:A:GLY:H	1:36:A:THR:HG23	13	0.27
(1,597)	1:36:A:THR:HG21	1:42:A:TYR:HB3	6	0.27
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	7	0.27
(1,592)	1:36:A:THR:HB	1:44:A:ALA:HB3	15	0.27
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	16	0.27
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	15	0.27
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	14	0.27
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	17	0.27
(1,511)	1:31:A:CYS:HB2	1:40:A:CYS:HA	20	0.27
(1,493)	1:29:A:CYS:HA	1:30:A:TYR:HD1	14	0.27
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	14	0.27
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	16	0.27
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	6	0.27
(1,307)	1:18:A:THR:HG22	1:30:A:TYR:HE1	3	0.27
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	4	0.27
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	8	0.27
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	14	0.27
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	16	0.27
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	19	0.27
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	20	0.27
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	7	0.27
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	12	0.27
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	13	0.27
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	7	0.27
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	11	0.27
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	13	0.27
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	14	0.27
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	20	0.27
(1,150)	1:6:A:ASN:HA	1:21:A:LYS:HG3	16	0.27
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	9	0.27
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	10	0.27
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	11	0.27
(1,85)	1:3:A:TYR:HA	1:2:A:VAL:HG21	12	0.27
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	19	0.27
(1,48)	1:24:A:LEU:HB3	1:25:A:TYR:HE1	11	0.27
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	3	0.27
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	6	0.27
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	7	0.27
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	2	0.27
(1,6)	1:7:A:PRO:HD2	1:21:A:LYS:HE3	17	0.27
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	17	0.26
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	19	0.26
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	13	0.26
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	16	0.26
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	19	0.26
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	5	0.26
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	3	0.26
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	11	0.26
(1,1620)	1:31:A:CYS:H	1:18:A:THR:HB	7	0.26
(1,1619)	1:31:A:CYS:H	1:30:A:TYR:HB2	2	0.26
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	17	0.26
(1,1512)	1:6:A:ASN:H	1:6:A:ASN:HB3	7	0.26
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	11	0.26
(1,1477)	1:18:A:THR:HG22	1:19:A:CYS:HB3	3	0.26
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	16	0.26
(1,1456)	1:32:A:ARG:HD2	1:31:A:CYS:HA	17	0.26
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	18	0.26
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	16	0.26
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	16	0.26
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	3	0.26
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	10	0.26
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	14	0.26
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	16	0.26
(1,1398)	1:78:A:CYS:HA	1:69:A:CYS:HB3	20	0.26
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	11	0.26
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	8	0.26
(1,1370)	1:83:A:TYR:H	1:82:A:LYS:HB3	7	0.26
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	4	0.26
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	6	0.26
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	18	0.26
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD12	3	0.26
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD13	8	0.26
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD13	12	0.26
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD12	16	0.26
(1,1317)	1:80:A:LEU:HD22	1:80:A:LEU:HD13	17	0.26
(1,1317)	1:80:A:LEU:HD22	1:80:A:LEU:HD13	18	0.26
(1,1317)	1:80:A:LEU:HD21	1:80:A:LEU:HD13	19	0.26
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	8	0.26
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	8	0.26
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	17	0.26
(1,1264)	1:78:A:CYS:HB3	1:51:A:LEU:H	9	0.26
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	2	0.26
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	12	0.26
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD12	12	0.26
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	2	0.26
(1,1140)	1:69:A:CYS:HB2	1:70:A:PRO:HD2	16	0.26
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	1	0.26
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	3	0.26
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	7	0.26
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	15	0.26
(1,1104)	1:69:A:CYS:HB3	1:54:A:GLY:HA3	20	0.26
(1,1103)	1:69:A:CYS:HB2	1:78:A:CYS:HA	9	0.26
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	1	0.26
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	7	0.26
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	14	0.26
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	3	0.26
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	13	0.26
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	3	0.26
(1,983)	1:62:A:TYR:HA	1:59:A:VAL:HG13	11	0.26
(1,958)	1:66:A:LYS:H	1:59:A:VAL:HG11	14	0.26
(1,938)	1:59:A:VAL:HG13	1:59:A:VAL:HG21	10	0.26
(1,938)	1:59:A:VAL:HG11	1:59:A:VAL:HG21	13	0.26
(1,938)	1:59:A:VAL:HG12	1:59:A:VAL:HG22	14	0.26
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	17	0.26
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	8	0.26
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	9	0.26
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	10	0.26
(1,872)	1:55:A:THR:HG21	1:67:A:CYS:HA	8	0.26
(1,816)	1:51:A:LEU:HB3	1:52:A:ASN:HA	5	0.26
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	19	0.26
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	10	0.26
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	14	0.26
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	16	0.26
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	17	0.26
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	15	0.26
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	20	0.26
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	12	0.26
(1,751)	1:47:A:PRO:HD3	1:47:A:PRO:HG2	1	0.26
(1,751)	1:47:A:PRO:HD3	1:47:A:PRO:HG2	3	0.26
(1,751)	1:47:A:PRO:HD3	1:47:A:PRO:HG2	8	0.26
(1,751)	1:47:A:PRO:HD3	1:47:A:PRO:HG2	9	0.26
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	7	0.26
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	12	0.26
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	20	0.26
(1,705)	1:44:A:ALA:HB3	1:65:A:TYR:HA	8	0.26
(1,699)	1:44:A:ALA:HB1	1:64:A:TYR:HB3	14	0.26
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	2	0.26
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	20	0.26
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	11	0.26
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	10	0.26
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	4	0.26
(1,532)	1:32:A:ARG:HD2	1:32:A:ARG:H	2	0.26
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	10	0.26
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	20	0.26
(1,393)	1:22:A:ARG:HG3	1:28:A:LYS:H	13	0.26
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	2	0.26
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	19	0.26
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	6	0.26
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	14	0.26
(1,304)	1:18:A:THR:HG22	1:30:A:TYR:HB2	2	0.26
(1,304)	1:18:A:THR:HG22	1:30:A:TYR:HB2	3	0.26
(1,283)	1:18:A:THR:HA	1:19:A:CYS:HB3	13	0.26
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	8	0.26
(1,219)	1:11:A:TYR:H	1:10:A:PRO:HB2	20	0.26
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	1	0.26
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	4	0.26
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	5	0.26
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	6	0.26
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	8	0.26
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	9	0.26
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	10	0.26
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	12	0.26
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	15	0.26
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	17	0.26
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	18	0.26
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	9	0.26
(1,122)	1:5:A:PRO:HB3	1:3:A:TYR:HE1	9	0.26
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	19	0.26
(1,66)	1:74:A:TYR:HD1	1:72:A:GLY:H	6	0.26
(1,59)	1:71:A:TYR:HD1	1:71:A:TYR:HB2	7	0.26
(1,59)	1:71:A:TYR:HD1	1:71:A:TYR:HB2	14	0.26
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	11	0.26
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	16	0.26
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	5	0.26
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	18	0.25
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	3	0.25
(1,1853)	1:81:A:LYS:H	1:81:A:LYS:HG2	10	0.25
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	13	0.25
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	19	0.25
(1,1769)	1:62:A:TYR:H	1:61:A:GLY:HA2	13	0.25
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	18	0.25
(1,1696)	1:44:A:ALA:H	1:43:A:ASN:HB2	10	0.25
(1,1696)	1:44:A:ALA:H	1:43:A:ASN:HB2	17	0.25
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	4	0.25
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	20	0.25
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	16	0.25
(1,1603)	1:29:A:CYS:H	1:28:A:LYS:HE3	13	0.25
(1,1602)	1:29:A:CYS:H	1:28:A:LYS:HD2	7	0.25
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	4	0.25
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	19	0.25
(1,1510)	1:6:A:ASN:H	1:5:A:PRO:HB2	19	0.25
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	14	0.25
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	3	0.25
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	8	0.25
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	18	0.25
(1,1426)	1:53:A:GLY:HA2	1:52:A:ASN:H	3	0.25
(1,1419)	1:60:A:TYR:HA	1:59:A:VAL:HG21	14	0.25
(1,1417)	1:63:A:PRO:HB2	1:64:A:TYR:HD1	6	0.25
(1,1417)	1:63:A:PRO:HB2	1:64:A:TYR:HD1	20	0.25
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	18	0.25
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	2	0.25
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	9	0.25
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	17	0.25
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	3	0.25
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	15	0.25
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD11	2	0.25
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD12	7	0.25
(1,1317)	1:80:A:LEU:HD21	1:80:A:LEU:HD11	11	0.25
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD13	14	0.25
(1,1317)	1:80:A:LEU:HD21	1:80:A:LEU:HD11	15	0.25
(1,1281)	1:79:A:GLN:HG2	1:80:A:LEU:HB2	6	0.25
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	15	0.25
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	3	0.25
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	13	0.25
(1,1240)	1:77:A:GLN:HB2	1:50:A:CYS:HA	14	0.25
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	14	0.25
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	17	0.25
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	13	0.25
(1,1133)	1:71:A:TYR:H	1:70:A:PRO:HB2	12	0.25
(1,1131)	1:70:A:PRO:HB3	1:73:A:TYR:HD1	4	0.25
(1,1131)	1:70:A:PRO:HB3	1:73:A:TYR:HD1	11	0.25
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	12	0.25
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	2	0.25
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	8	0.25
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	10	0.25
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	14	0.25
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	5	0.25
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	14	0.25
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	20	0.25
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	8	0.25
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	10	0.25
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG12	12	0.25
(1,960)	1:59:A:VAL:HG22	1:60:A:TYR:HB2	12	0.25
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	4	0.25
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	11	0.25
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	19	0.25
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	3	0.25
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	13	0.25
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	18	0.25
(1,875)	1:68:A:SER:H	1:55:A:THR:HG23	13	0.25
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	12	0.25
(1,849)	1:54:A:GLY:HA2	1:70:A:PRO:HD2	4	0.25
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	18	0.25
(1,804)	1:51:A:LEU:H	1:50:A:CYS:HB3	10	0.25
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	10	0.25
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	3	0.25
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	8	0.25
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	11	0.25
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	13	0.25
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	15	0.25
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	18	0.25
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	20	0.25
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	1	0.25
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	13	0.25
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	4	0.25
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	11	0.25
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:47:A:PRO:HD3	1:47:A:PRO:HG2	19	0.25
(1,747)	1:48:A:ASN:H	1:47:A:PRO:HB2	19	0.25
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	4	0.25
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	6	0.25
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	10	0.25
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	14	0.25
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	15	0.25
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	16	0.25
(1,705)	1:44:A:ALA:HB3	1:65:A:TYR:HA	17	0.25
(1,679)	1:43:A:ASN:HA	1:36:A:THR:HG21	3	0.25
(1,666)	1:40:A:CYS:HB2	1:39:A:ASN:HA	8	0.25
(1,664)	1:40:A:CYS:HB2	1:31:A:CYS:HA	8	0.25
(1,664)	1:40:A:CYS:HB2	1:31:A:CYS:HA	18	0.25
(1,641)	1:39:A:ASN:HA	1:29:A:CYS:HB3	13	0.25
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG21	15	0.25
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	14	0.25
(1,597)	1:36:A:THR:HG22	1:42:A:TYR:HB3	2	0.25
(1,573)	1:73:A:TYR:HA	1:81:A:LYS:HG2	3	0.25
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	19	0.25
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	12	0.25
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	2	0.25
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	17	0.25
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	19	0.25
(1,284)	1:18:A:THR:HA	1:19:A:CYS:HB2	14	0.25
(1,272)	1:17:A:GLY:HA2	1:18:A:THR:HB	7	0.25
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	14	0.25
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	16	0.25
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	16	0.25
(1,219)	1:11:A:TYR:H	1:10:A:PRO:HB2	7	0.25
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	14	0.25
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	16	0.25
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	19	0.25
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	17	0.25
(1,194)	1:8:A:CYS:HB2	1:7:A:PRO:HA	7	0.25
(1,175)	1:8:A:CYS:H	1:7:A:PRO:HD2	19	0.25
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	2	0.25
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	3	0.25
(1,117)	1:5:A:PRO:HB2	1:5:A:PRO:HD2	4	0.25
(1,114)	1:5:A:PRO:HA	1:3:A:TYR:HD1	12	0.25
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	15	0.25
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	5	0.25
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:71:A:TYR:HD1	1:71:A:TYR:HB2	9	0.25
(1,59)	1:71:A:TYR:HD1	1:71:A:TYR:HB2	10	0.25
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	4	0.25
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	10	0.25
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	18	0.25
(1,35)	1:80:A:LEU:H	1:79:A:GLN:HB2	1	0.25
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	16	0.25
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	10	0.24
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	12	0.24
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	19	0.24
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	17	0.24
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	8	0.24
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	16	0.24
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	6	0.24
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	2	0.24
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	16	0.24
(1,1762)	1:61:A:GLY:H	1:60:A:TYR:HB2	16	0.24
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	6	0.24
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	2	0.24
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	5	0.24
(1,1709)	1:46:A:PHE:H	1:46:A:PHE:HD1	10	0.24
(1,1676)	1:79:A:GLN:H	1:75:A:GLY:HA2	16	0.24
(1,1635)	1:34:A:GLY:H	1:33:A:LYS:HB3	8	0.24
(1,1540)	1:17:A:GLY:H	1:13:A:CYS:HB2	13	0.24
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	3	0.24
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	10	0.24
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	15	0.24
(1,1527)	1:14:A:ARG:H	1:39:A:ASN:HA	16	0.24
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	20	0.24
(1,1500)	1:51:A:LEU:HD22	1:50:A:CYS:H	7	0.24
(1,1489)	1:3:A:TYR:HB2	1:4:A:TYR:H	18	0.24
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	19	0.24
(1,1477)	1:18:A:THR:HG21	1:19:A:CYS:HB3	10	0.24
(1,1433)	1:47:A:PRO:HG3	1:46:A:PHE:HD1	3	0.24
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	4	0.24
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	12	0.24
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	7	0.24
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	17	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	1	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	2	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	3	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	6	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	8	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	9	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	10	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	11	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	12	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	13	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	14	0.24
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	20	0.24
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	2	0.24
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	5	0.24
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	10	0.24
(1,1347)	1:82:A:LYS:HA	1:82:A:LYS:HG2	20	0.24
(1,1317)	1:80:A:LEU:HD22	1:80:A:LEU:HD13	1	0.24
(1,1309)	1:79:A:GLN:HG3	1:80:A:LEU:HD13	17	0.24
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	16	0.24
(1,1227)	1:5:A:PRO:HB2	1:3:A:TYR:HE1	2	0.24
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD13	2	0.24
(1,1216)	1:77:A:GLN:H	1:75:A:GLY:HA2	3	0.24
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	5	0.24
(1,1183)	1:72:A:GLY:HA3	1:73:A:TYR:HE1	11	0.24
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	7	0.24
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	7	0.24
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	12	0.24
(1,1159)	1:70:A:PRO:HG3	1:55:A:THR:H	4	0.24
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	8	0.24
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	3	0.24
(1,1133)	1:71:A:TYR:H	1:70:A:PRO:HB2	5	0.24
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	10	0.24
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	16	0.24
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	18	0.24
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	6	0.24
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	11	0.24
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	13	0.24
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	14	0.24
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	17	0.24
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	19	0.24
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	7	0.24
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	20	0.24
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	18	0.24
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	18	0.24
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	6	0.24
(1,1074)	1:56:A:CYS:HB2	1:67:A:CYS:HA	16	0.24
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	15	0.24
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	16	0.24
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	11	0.24
(1,1036)	1:59:A:VAL:HG13	1:65:A:TYR:HA	7	0.24
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG12	8	0.24
(1,953)	1:59:A:VAL:HG13	1:60:A:TYR:HD1	14	0.24
(1,938)	1:59:A:VAL:HG11	1:59:A:VAL:HG21	3	0.24
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	15	0.24
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	16	0.24
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	17	0.24
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	6	0.24
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	15	0.24
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	1	0.24
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	12	0.24
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	12	0.24
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	15	0.24
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	14	0.24
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	16	0.24
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	8	0.24
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	2	0.24
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	5	0.24
(1,740)	1:47:A:PRO:HA	1:47:A:PRO:HD2	13	0.24
(1,704)	1:44:A:ALA:HB3	1:35:A:TYR:HA	1	0.24
(1,688)	1:44:A:ALA:HA	1:36:A:THR:HG21	17	0.24
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	4	0.24
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	7	0.24
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	18	0.24
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	4	0.24
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	10	0.24
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	5	0.24
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	10	0.24
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	12	0.24
(1,486)	1:28:A:LYS:HB3	1:28:A:LYS:H	6	0.24
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	13	0.24
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	5	0.24
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	9	0.24
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	10	0.24
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	16	0.24
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	3	0.24
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	10	0.24
(1,237)	1:11:A:TYR:HB3	1:11:A:TYR:H	7	0.24
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	3	0.24
(1,212)	1:10:A:PRO:HA	1:9:A:SER:H	14	0.24
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	19	0.24
(1,177)	1:7:A:PRO:HG2	1:27:A:TYR:HB2	10	0.24
(1,59)	1:71:A:TYR:HD1	1:71:A:TYR:HB2	11	0.24
(1,59)	1:71:A:TYR:HD1	1:71:A:TYR:HB2	20	0.24
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	7	0.24
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	13	0.24
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	18	0.24
(1,48)	1:24:A:LEU:HB3	1:25:A:TYR:HE1	6	0.24
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	14	0.24
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	18	0.24
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	18	0.23
(1,1886)	1:22:A:ARG:H	1:27:A:TYR:HD1	3	0.23
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	3	0.23
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	14	0.23
(1,1842)	1:78:A:CYS:H	1:80:A:LEU:HD12	1	0.23
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	14	0.23
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	16	0.23
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	6	0.23
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	15	0.23
(1,1776)	1:65:A:TYR:H	1:59:A:VAL:HB	7	0.23
(1,1776)	1:65:A:TYR:H	1:59:A:VAL:HB	12	0.23
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	6	0.23
(1,1696)	1:44:A:ALA:H	1:43:A:ASN:HB2	9	0.23
(1,1696)	1:44:A:ALA:H	1:43:A:ASN:HB2	18	0.23
(1,1683)	1:42:A:TYR:H	1:42:A:TYR:HB3	6	0.23
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	6	0.23
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	11	0.23
(1,1676)	1:79:A:GLN:H	1:75:A:GLY:HA2	14	0.23
(1,1671)	1:41:A:GLN:H	1:39:A:ASN:HB3	3	0.23
(1,1619)	1:31:A:CYS:H	1:30:A:TYR:HB2	9	0.23
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	12	0.23
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD12	7	0.23
(1,1579)	1:24:A:LEU:H	1:25:A:TYR:HA	7	0.23
(1,1571)	1:82:A:LYS:H	1:74:A:TYR:HD1	15	0.23
(1,1539)	1:17:A:GLY:H	1:32:A:ARG:HG2	14	0.23
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	1	0.23
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	5	0.23
(1,1512)	1:6:A:ASN:H	1:6:A:ASN:HB3	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	14	0.23
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	6	0.23
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	8	0.23
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	17	0.23
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	18	0.23
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	8	0.23
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	5	0.23
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	6	0.23
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	5	0.23
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	8	0.23
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	17	0.23
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	14	0.23
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	6	0.23
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	6	0.23
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	14	0.23
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	5	0.23
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	7	0.23
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	15	0.23
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	16	0.23
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	18	0.23
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	19	0.23
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	17	0.23
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	1	0.23
(1,1343)	1:81:A:LYS:HD2	1:73:A:TYR:HA	2	0.23
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	14	0.23
(1,1319)	1:79:A:GLN:HG3	1:80:A:LEU:HD23	17	0.23
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	12	0.23
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	14	0.23
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	14	0.23
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	2	0.23
(1,1219)	1:76:A:LYS:HA	1:80:A:LEU:HD13	11	0.23
(1,1146)	1:70:A:PRO:HD2	1:73:A:TYR:HA	12	0.23
(1,1131)	1:70:A:PRO:HB3	1:73:A:TYR:HD1	12	0.23
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	19	0.23
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	1	0.23
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	15	0.23
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	9	0.23
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	16	0.23
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	12	0.23
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	2	0.23
(1,1086)	1:68:A:SER:HB3	1:69:A:CYS:H	6	0.23
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1064)	1:66:A:LYS:HG3	1:59:A:VAL:HG21	13	0.23
(1,1055)	1:66:A:LYS:H	1:65:A:TYR:HB3	11	0.23
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	5	0.23
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	8	0.23
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	2	0.23
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	11	0.23
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	12	0.23
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	14	0.23
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	15	0.23
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	17	0.23
(1,994)	1:63:A:PRO:HA	1:63:A:PRO:HG3	18	0.23
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG13	12	0.23
(1,951)	1:65:A:TYR:H	1:59:A:VAL:HG12	17	0.23
(1,940)	1:59:A:VAL:HG11	1:66:A:LYS:HG2	7	0.23
(1,938)	1:59:A:VAL:HG13	1:59:A:VAL:HG21	5	0.23
(1,938)	1:59:A:VAL:HG13	1:59:A:VAL:HG23	17	0.23
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	1	0.23
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	2	0.23
(1,875)	1:68:A:SER:H	1:55:A:THR:HG21	4	0.23
(1,872)	1:55:A:THR:HG22	1:67:A:CYS:HA	17	0.23
(1,826)	1:51:A:LEU:HD11	1:51:A:LEU:HD23	1	0.23
(1,826)	1:51:A:LEU:HD12	1:51:A:LEU:HD23	4	0.23
(1,826)	1:51:A:LEU:HD11	1:51:A:LEU:HD23	5	0.23
(1,826)	1:51:A:LEU:HD11	1:51:A:LEU:HD22	14	0.23
(1,826)	1:51:A:LEU:HD13	1:51:A:LEU:HD23	17	0.23
(1,826)	1:51:A:LEU:HD12	1:51:A:LEU:HD21	19	0.23
(1,826)	1:51:A:LEU:HD12	1:51:A:LEU:HD22	20	0.23
(1,824)	1:51:A:LEU:HD23	1:51:A:LEU:H	12	0.23
(1,804)	1:51:A:LEU:H	1:50:A:CYS:HB3	16	0.23
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	10	0.23
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	14	0.23
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	18	0.23
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	6	0.23
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	9	0.23
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	1	0.23
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	3	0.23
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	2	0.23
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	6	0.23
(1,677)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	18	0.23
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	15	0.23
(1,600)	1:36:A:THR:HG23	1:64:A:TYR:HB2	14	0.23
(1,592)	1:36:A:THR:HB	1:44:A:ALA:HB3	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,558)	1:33:A:LYS:H	1:33:A:LYS:HG2	11	0.23
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	4	0.23
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	19	0.23
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	20	0.23
(1,493)	1:29:A:CYS:HA	1:30:A:TYR:HD1	1	0.23
(1,489)	1:29:A:CYS:HA	1:18:A:THR:HG21	1	0.23
(1,488)	1:28:A:LYS:HE2	1:28:A:LYS:HA	6	0.23
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	17	0.23
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	9	0.23
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	18	0.23
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD12	9	0.23
(1,391)	1:22:A:ARG:HG3	1:27:A:TYR:HA	11	0.23
(1,366)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	20	0.23
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	2	0.23
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	12	0.23
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	19	0.23
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	17	0.23
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	18	0.23
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	8	0.23
(1,327)	1:20:A:LYS:HB3	1:30:A:TYR:HE1	17	0.23
(1,313)	1:19:A:CYS:HB3	1:29:A:CYS:HA	13	0.23
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	1	0.23
(1,237)	1:11:A:TYR:HB3	1:11:A:TYR:H	13	0.23
(1,234)	1:11:A:TYR:HA	1:11:A:TYR:HE1	1	0.23
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	15	0.23
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	4	0.23
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	7	0.23
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	14	0.23
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	6	0.23
(1,188)	1:8:A:CYS:HA	1:9:A:SER:HB2	13	0.23
(1,175)	1:8:A:CYS:H	1:7:A:PRO:HD2	15	0.23
(1,121)	1:5:A:PRO:HB3	1:4:A:TYR:HA	2	0.23
(1,107)	1:4:A:TYR:H	1:4:A:TYR:HB3	9	0.23
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	5	0.23
(1,59)	1:71:A:TYR:HD1	1:71:A:TYR:HB2	6	0.23
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	1	0.23
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	6	0.23
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	12	0.23
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	2	0.22
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	14	0.22
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	11	0.22
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1869)	1:53:A:GLY:H	1:51:A:LEU:HD22	1	0.22
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	11	0.22
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	8	0.22
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	18	0.22
(1,1815)	1:74:A:TYR:H	1:81:A:LYS:HB3	17	0.22
(1,1810)	1:73:A:TYR:H	1:81:A:LYS:HA	3	0.22
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	3	0.22
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	7	0.22
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	2	0.22
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	4	0.22
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	9	0.22
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	14	0.22
(1,1740)	1:57:A:GLY:H	1:66:A:LYS:HB2	19	0.22
(1,1714)	1:50:A:CYS:H	1:49:A:PRO:HG2	19	0.22
(1,1698)	1:44:A:ALA:H	1:58:A:TYR:HE1	1	0.22
(1,1671)	1:41:A:GLN:H	1:39:A:ASN:HB3	15	0.22
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	1	0.22
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	9	0.22
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	2	0.22
(1,1572)	1:23:A:GLY:H	1:22:A:ARG:HB2	17	0.22
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	2	0.22
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	4	0.22
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	9	0.22
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	3	0.22
(1,1477)	1:18:A:THR:HG22	1:19:A:CYS:HB3	7	0.22
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	5	0.22
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	18	0.22
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	10	0.22
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	10	0.22
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	13	0.22
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	18	0.22
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	15	0.22
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	8	0.22
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	9	0.22
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	11	0.22
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	20	0.22
(1,1357)	1:82:A:LYS:HB2	1:82:A:LYS:HG2	1	0.22
(1,1357)	1:82:A:LYS:HB2	1:82:A:LYS:HG2	7	0.22
(1,1357)	1:82:A:LYS:HB2	1:82:A:LYS:HG2	12	0.22
(1,1357)	1:82:A:LYS:HB2	1:82:A:LYS:HG2	13	0.22
(1,1357)	1:82:A:LYS:HB2	1:82:A:LYS:HG2	17	0.22
(1,1357)	1:82:A:LYS:HB2	1:82:A:LYS:HG2	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1317)	1:80:A:LEU:HD23	1:80:A:LEU:HD13	9	0.22
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	6	0.22
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	8	0.22
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	20	0.22
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	1	0.22
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	3	0.22
(1,1228)	1:75:A:GLY:HA3	1:76:A:LYS:HG3	15	0.22
(1,1228)	1:75:A:GLY:HA3	1:76:A:LYS:HG3	17	0.22
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	3	0.22
(1,1191)	1:73:A:TYR:HB3	1:70:A:PRO:HD3	6	0.22
(1,1131)	1:70:A:PRO:HB3	1:73:A:TYR:HD1	20	0.22
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	2	0.22
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	7	0.22
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	8	0.22
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	9	0.22
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	13	0.22
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	20	0.22
(1,1111)	1:69:A:CYS:H	1:69:A:CYS:HB3	4	0.22
(1,1103)	1:69:A:CYS:HB2	1:78:A:CYS:HA	6	0.22
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	8	0.22
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	11	0.22
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	7	0.22
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	4	0.22
(1,1069)	1:66:A:LYS:HG3	1:66:A:LYS:H	3	0.22
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	2	0.22
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	16	0.22
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	19	0.22
(1,1030)	1:64:A:TYR:HB3	1:65:A:TYR:HB3	12	0.22
(1,1010)	1:63:A:PRO:HD2	1:64:A:TYR:H	20	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	1	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	3	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	4	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	5	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	6	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	7	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	9	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	13	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	16	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	18	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	19	0.22
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	20	0.22
(1,994)	1:63:A:PRO:HA	1:63:A:PRO:HG3	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	14	0.22
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG12	5	0.22
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	6	0.22
(1,903)	1:58:A:TYR:HA	1:66:A:LYS:HB2	6	0.22
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	10	0.22
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	5	0.22
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	14	0.22
(1,875)	1:68:A:SER:H	1:55:A:THR:HG21	6	0.22
(1,872)	1:55:A:THR:HG21	1:67:A:CYS:HA	7	0.22
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	2	0.22
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	5	0.22
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	7	0.22
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	10	0.22
(1,826)	1:51:A:LEU:HD11	1:51:A:LEU:HD21	2	0.22
(1,826)	1:51:A:LEU:HD13	1:51:A:LEU:HD21	7	0.22
(1,826)	1:51:A:LEU:HD13	1:51:A:LEU:HD22	9	0.22
(1,826)	1:51:A:LEU:HD13	1:51:A:LEU:HD22	16	0.22
(1,826)	1:51:A:LEU:HD13	1:51:A:LEU:HD23	18	0.22
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	12	0.22
(1,804)	1:51:A:LEU:H	1:50:A:CYS:HB3	4	0.22
(1,796)	1:50:A:CYS:HA	1:78:A:CYS:HB3	2	0.22
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	3	0.22
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	4	0.22
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	6	0.22
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	11	0.22
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	16	0.22
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	20	0.22
(1,757)	1:48:A:ASN:H	1:47:A:PRO:HD3	18	0.22
(1,704)	1:44:A:ALA:HB3	1:35:A:TYR:HA	10	0.22
(1,704)	1:44:A:ALA:HB2	1:35:A:TYR:HA	13	0.22
(1,699)	1:44:A:ALA:HB3	1:64:A:TYR:HB3	15	0.22
(1,697)	1:44:A:ALA:HB1	1:34:A:GLY:HA2	5	0.22
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	11	0.22
(1,664)	1:40:A:CYS:HB2	1:31:A:CYS:HA	7	0.22
(1,632)	1:66:A:LYS:HE2	1:59:A:VAL:HG22	7	0.22
(1,603)	1:36:A:THR:HG21	1:42:A:TYR:HA	15	0.22
(1,588)	1:58:A:TYR:HB2	1:59:A:VAL:H	20	0.22
(1,566)	1:34:A:GLY:HA3	1:58:A:TYR:HD1	2	0.22
(1,565)	1:34:A:GLY:HA3	1:35:A:TYR:HD1	8	0.22
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	10	0.22
(1,510)	1:31:A:CYS:HB2	1:40:A:CYS:HB2	7	0.22
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:30:A:TYR:HA	1:30:A:TYR:HD1	12	0.22
(1,490)	1:29:A:CYS:HA	1:20:A:LYS:HG2	5	0.22
(1,477)	1:28:A:LYS:HB2	1:28:A:LYS:HE3	2	0.22
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	15	0.22
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	15	0.22
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD11	2	0.22
(1,367)	1:27:A:TYR:HB2	1:27:A:TYR:HD1	13	0.22
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	4	0.22
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	15	0.22
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	14	0.22
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	13	0.22
(1,308)	1:18:A:THR:HG21	1:30:A:TYR:HD1	9	0.22
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	16	0.22
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	5	0.22
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	12	0.22
(1,230)	1:10:A:PRO:HG3	1:11:A:TYR:H	4	0.22
(1,224)	1:10:A:PRO:HD2	1:11:A:TYR:H	20	0.22
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	18	0.22
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	13	0.22
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	14	0.22
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	18	0.22
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	19	0.22
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	2	0.22
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	2	0.22
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	2	0.22
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	4	0.22
(1,181)	1:7:A:PRO:HG2	1:27:A:TYR:HA	19	0.22
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	19	0.22
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	14	0.22
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	16	0.22
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	13	0.22
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	14	0.22
(1,59)	1:71:A:TYR:HD1	1:71:A:TYR:HB2	5	0.22
(1,53)	1:58:A:TYR:HE1	1:44:A:ALA:HA	5	0.22
(1,38)	1:82:A:LYS:H	1:74:A:TYR:HE1	14	0.22
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	2	0.22
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	17	0.22
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	11	0.22
(1,17)	1:54:A:GLY:HA2	1:53:A:GLY:HA2	12	0.22
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	3	0.21
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	19	0.21
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1844)	1:78:A:CYS:H	1:74:A:TYR:HA	15	0.21
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	15	0.21
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	16	0.21
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	7	0.21
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	11	0.21
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	3	0.21
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	20	0.21
(1,1740)	1:57:A:GLY:H	1:66:A:LYS:HB2	12	0.21
(1,1703)	1:45:A:CYS:H	1:58:A:TYR:HD1	7	0.21
(1,1703)	1:45:A:CYS:H	1:58:A:TYR:HD1	10	0.21
(1,1696)	1:44:A:ALA:H	1:43:A:ASN:HB2	12	0.21
(1,1696)	1:44:A:ALA:H	1:43:A:ASN:HB2	19	0.21
(1,1683)	1:42:A:TYR:H	1:42:A:TYR:HB3	9	0.21
(1,1676)	1:79:A:GLN:H	1:75:A:GLY:HA2	17	0.21
(1,1666)	1:79:A:GLN:H	1:80:A:LEU:HD11	3	0.21
(1,1658)	1:39:A:ASN:H	1:41:A:GLN:H	2	0.21
(1,1641)	1:35:A:TYR:H	1:35:A:TYR:HE1	8	0.21
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	17	0.21
(1,1603)	1:29:A:CYS:H	1:28:A:LYS:HE3	2	0.21
(1,1602)	1:29:A:CYS:H	1:28:A:LYS:HD2	14	0.21
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	13	0.21
(1,1572)	1:23:A:GLY:H	1:22:A:ARG:HB2	4	0.21
(1,1527)	1:14:A:ARG:H	1:39:A:ASN:HA	12	0.21
(1,1504)	1:3:A:TYR:H	1:2:A:VAL:HB	12	0.21
(1,1503)	1:2:A:VAL:H	1:2:A:VAL:HB	10	0.21
(1,1477)	1:18:A:THR:HG21	1:19:A:CYS:HB3	4	0.21
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	10	0.21
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	11	0.21
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	12	0.21
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	15	0.21
(1,1398)	1:78:A:CYS:HA	1:69:A:CYS:HB3	9	0.21
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	5	0.21
(1,1391)	1:83:A:TYR:H	1:83:A:TYR:HA	17	0.21
(1,1357)	1:82:A:LYS:HB2	1:82:A:LYS:HG2	19	0.21
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	8	0.21
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	1	0.21
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	5	0.21
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	4	0.21
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	10	0.21
(1,1226)	1:76:A:LYS:HA	1:75:A:GLY:H	15	0.21
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	5	0.21
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	11	0.21
(1,1131)	1:70:A:PRO:HB3	1:73:A:TYR:HD1	18	0.21
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	5	0.21
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	17	0.21
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	18	0.21
(1,1092)	1:69:A:CYS:HA	1:55:A:THR:HB	13	0.21
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	2	0.21
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	9	0.21
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	13	0.21
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	15	0.21
(1,1047)	1:58:A:TYR:H	1:65:A:TYR:HA	18	0.21
(1,1046)	1:59:A:VAL:H	1:65:A:TYR:HA	12	0.21
(1,1036)	1:59:A:VAL:HG12	1:65:A:TYR:HA	6	0.21
(1,1002)	1:63:A:PRO:HB3	1:63:A:PRO:HD2	10	0.21
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG13	1	0.21
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG12	4	0.21
(1,960)	1:59:A:VAL:HG21	1:60:A:TYR:HB2	7	0.21
(1,958)	1:66:A:LYS:H	1:59:A:VAL:HG11	1	0.21
(1,958)	1:66:A:LYS:H	1:59:A:VAL:HG13	15	0.21
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG13	13	0.21
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	14	0.21
(1,826)	1:51:A:LEU:HD11	1:51:A:LEU:HD22	8	0.21
(1,826)	1:51:A:LEU:HD11	1:51:A:LEU:HD21	10	0.21
(1,826)	1:51:A:LEU:HD12	1:51:A:LEU:HD21	11	0.21
(1,826)	1:51:A:LEU:HD13	1:51:A:LEU:HD22	12	0.21
(1,826)	1:51:A:LEU:HD13	1:51:A:LEU:HD22	15	0.21
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	14	0.21
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	8	0.21
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	9	0.21
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	17	0.21
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	17	0.21
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	4	0.21
(1,707)	1:44:A:ALA:HB1	1:58:A:TYR:HD1	5	0.21
(1,664)	1:40:A:CYS:HB2	1:31:A:CYS:HA	17	0.21
(1,623)	1:38:A:LYS:HB3	1:38:A:LYS:HE2	4	0.21
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	4	0.21
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	6	0.21
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	11	0.21
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	18	0.21
(1,569)	1:34:A:GLY:HA2	1:58:A:TYR:HD1	12	0.21
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	2	0.21
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	3	0.21
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	6	0.21
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	19	0.21
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	8	0.21
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	14	0.21
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	17	0.21
(1,393)	1:22:A:ARG:HG3	1:28:A:LYS:H	15	0.21
(1,392)	1:22:A:ARG:HG3	1:22:A:ARG:H	7	0.21
(1,392)	1:22:A:ARG:HG3	1:22:A:ARG:H	20	0.21
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	3	0.21
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	1	0.21
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	3	0.21
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	11	0.21
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	7	0.21
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	1	0.21
(1,336)	1:20:A:LYS:HB2	1:21:A:LYS:H	7	0.21
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	7	0.21
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	14	0.21
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	15	0.21
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	7	0.21
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	2	0.21
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	13	0.21
(1,247)	1:13:A:CYS:HB2	1:31:A:CYS:HA	14	0.21
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	4	0.21
(1,237)	1:11:A:TYR:HB3	1:11:A:TYR:H	20	0.21
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	1	0.21
(1,219)	1:11:A:TYR:H	1:10:A:PRO:HB2	8	0.21
(1,219)	1:11:A:TYR:H	1:10:A:PRO:HB2	17	0.21
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	18	0.21
(1,199)	1:9:A:SER:H	1:9:A:SER:HB3	15	0.21
(1,199)	1:9:A:SER:H	1:9:A:SER:HB3	20	0.21
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	3	0.21
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	7	0.21
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	18	0.21
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	8	0.21
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	13	0.21
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	18	0.21
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	16	0.21
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	8	0.21
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	2	0.21
(1,83)	1:2:A:VAL:HG21	1:4:A:TYR:HE1	17	0.21
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	14	0.21
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	7	0.21
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE2	4	0.21
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	11	0.2
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	13	0.2
(1,1886)	1:22:A:ARG:H	1:27:A:TYR:HD1	19	0.2
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	2	0.2
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	6	0.2
(1,1831)	1:76:A:LYS:H	1:76:A:LYS:HE2	18	0.2
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	19	0.2
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	8	0.2
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	9	0.2
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	10	0.2
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	17	0.2
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	7	0.2
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	13	0.2
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	1	0.2
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	10	0.2
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	20	0.2
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	12	0.2
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	8	0.2
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	10	0.2
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	14	0.2
(1,1636)	1:34:A:GLY:H	1:35:A:TYR:HD1	5	0.2
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	19	0.2
(1,1516)	1:8:A:CYS:H	1:7:A:PRO:HG3	7	0.2
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	2	0.2
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	4	0.2
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	16	0.2
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	19	0.2
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	4	0.2
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	18	0.2
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	10	0.2
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	2	0.2
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	10	0.2
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	17	0.2
(1,1404)	1:74:A:TYR:HA	1:73:A:TYR:HA	11	0.2
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	14	0.2
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	2	0.2
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	20	0.2
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	14	0.2
(1,1357)	1:82:A:LYS:HB2	1:82:A:LYS:HG2	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1347)	1:82:A:LYS:HA	1:82:A:LYS:HG2	17	0.2
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	12	0.2
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	13	0.2
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	10	0.2
(1,1159)	1:70:A:PRO:HG3	1:55:A:THR:H	7	0.2
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	6	0.2
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	14	0.2
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	12	0.2
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	4	0.2
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	3	0.2
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	12	0.2
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	12	0.2
(1,1036)	1:59:A:VAL:HG13	1:65:A:TYR:HA	19	0.2
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG11	6	0.2
(1,958)	1:66:A:LYS:H	1:59:A:VAL:HG11	11	0.2
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG13	8	0.2
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	15	0.2
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	12	0.2
(1,872)	1:55:A:THR:HG22	1:67:A:CYS:HA	14	0.2
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	1	0.2
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	20	0.2
(1,826)	1:51:A:LEU:HD11	1:51:A:LEU:HD22	3	0.2
(1,826)	1:51:A:LEU:HD11	1:51:A:LEU:HD23	6	0.2
(1,826)	1:51:A:LEU:HD13	1:51:A:LEU:HD21	13	0.2
(1,824)	1:51:A:LEU:HD22	1:51:A:LEU:H	19	0.2
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	5	0.2
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	17	0.2
(1,770)	1:49:A:PRO:HA	1:49:A:PRO:HG2	7	0.2
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	7	0.2
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	12	0.2
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	13	0.2
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	15	0.2
(1,756)	1:47:A:PRO:HD2	1:48:A:ASN:H	5	0.2
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	2	0.2
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	5	0.2
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	7	0.2
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	10	0.2
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	12	0.2
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	13	0.2
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	16	0.2
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	17	0.2
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	14	0.2
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	15	0.2
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	17	0.2
(1,717)	1:45:A:CYS:HA	1:58:A:TYR:HE1	3	0.2
(1,699)	1:44:A:ALA:HB3	1:64:A:TYR:HB3	1	0.2
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	11	0.2
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	17	0.2
(1,614)	1:38:A:LYS:HA	1:38:A:LYS:HG2	16	0.2
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	13	0.2
(1,594)	1:36:A:THR:HB	1:64:A:TYR:HD1	8	0.2
(1,588)	1:58:A:TYR:HB2	1:59:A:VAL:H	16	0.2
(1,549)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	9	0.2
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	1	0.2
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	7	0.2
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	16	0.2
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	1	0.2
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	3	0.2
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	7	0.2
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	13	0.2
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	19	0.2
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	18	0.2
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	14	0.2
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	5	0.2
(1,314)	1:19:A:CYS:HB3	1:11:A:TYR:HE1	20	0.2
(1,262)	1:15:A:ASN:HB3	1:35:A:TYR:HD1	15	0.2
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	18	0.2
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	12	0.2
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	17	0.2
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	1	0.2
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	11	0.2
(1,150)	1:6:A:ASN:HA	1:21:A:LYS:HG3	11	0.2
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	5	0.2
(1,96)	1:3:A:TYR:HB2	1:3:A:TYR:H	20	0.2
(1,90)	1:4:A:TYR:H	1:3:A:TYR:HA	17	0.2
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	1	0.2
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	8	0.2
(1,62)	1:73:A:TYR:HD1	1:73:A:TYR:HA	12	0.2
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	15	0.2
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	17	0.2
(1,48)	1:24:A:LEU:HB3	1:25:A:TYR:HE1	8	0.2
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	1	0.2
(1,16)	1:54:A:GLY:HA3	1:55:A:THR:HB	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	6	0.19
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	3	0.19
(1,1844)	1:78:A:CYS:H	1:74:A:TYR:HA	13	0.19
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	13	0.19
(1,1809)	1:73:A:TYR:H	1:72:A:GLY:HA3	4	0.19
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	9	0.19
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	9	0.19
(1,1762)	1:61:A:GLY:H	1:60:A:TYR:HB2	9	0.19
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	10	0.19
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	3	0.19
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	12	0.19
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	18	0.19
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	19	0.19
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	11	0.19
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	19	0.19
(1,1703)	1:45:A:CYS:H	1:58:A:TYR:HD1	1	0.19
(1,1696)	1:44:A:ALA:H	1:43:A:ASN:HB2	20	0.19
(1,1666)	1:79:A:GLN:H	1:80:A:LEU:HD11	7	0.19
(1,1666)	1:79:A:GLN:H	1:80:A:LEU:HD11	16	0.19
(1,1658)	1:39:A:ASN:H	1:41:A:GLN:H	17	0.19
(1,1658)	1:39:A:ASN:H	1:41:A:GLN:H	18	0.19
(1,1640)	1:35:A:TYR:H	1:36:A:THR:HA	6	0.19
(1,1619)	1:31:A:CYS:H	1:30:A:TYR:HB2	16	0.19
(1,1603)	1:29:A:CYS:H	1:28:A:LYS:HE3	10	0.19
(1,1572)	1:23:A:GLY:H	1:22:A:ARG:HB2	14	0.19
(1,1571)	1:82:A:LYS:H	1:74:A:TYR:HD1	16	0.19
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	4	0.19
(1,1539)	1:17:A:GLY:H	1:32:A:ARG:HG2	19	0.19
(1,1500)	1:51:A:LEU:HD21	1:50:A:CYS:H	6	0.19
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	9	0.19
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	1	0.19
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	18	0.19
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	6	0.19
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	15	0.19
(1,1426)	1:53:A:GLY:HA2	1:52:A:ASN:H	13	0.19
(1,1417)	1:63:A:PRO:HB2	1:64:A:TYR:HD1	4	0.19
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	4	0.19
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	11	0.19
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	10	0.19
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	12	0.19
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	8	0.19
(1,1347)	1:82:A:LYS:HA	1:82:A:LYS:HG2	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1337)	1:81:A:LYS:HB2	1:83:A:TYR:HE1	14	0.19
(1,1332)	1:81:A:LYS:HB3	1:81:A:LYS:HE2	10	0.19
(1,1323)	1:80:A:LEU:H	1:80:A:LEU:HD21	10	0.19
(1,1281)	1:79:A:GLN:HG2	1:80:A:LEU:HB2	13	0.19
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	7	0.19
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	14	0.19
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	12	0.19
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	18	0.19
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	10	0.19
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	20	0.19
(1,1226)	1:76:A:LYS:HA	1:75:A:GLY:H	11	0.19
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	18	0.19
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	20	0.19
(1,1191)	1:73:A:TYR:HB3	1:70:A:PRO:HD3	1	0.19
(1,1134)	1:71:A:TYR:H	1:70:A:PRO:HB3	3	0.19
(1,1133)	1:71:A:TYR:H	1:70:A:PRO:HB2	17	0.19
(1,1129)	1:70:A:PRO:HB3	1:73:A:TYR:HE1	17	0.19
(1,1071)	1:67:A:CYS:HA	1:50:A:CYS:HB3	19	0.19
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	2	0.19
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	10	0.19
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	18	0.19
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	10	0.19
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	17	0.19
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	1	0.19
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	4	0.19
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	17	0.19
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	6	0.19
(1,989)	1:62:A:TYR:HA	1:61:A:GLY:H	6	0.19
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG12	7	0.19
(1,960)	1:59:A:VAL:HG22	1:60:A:TYR:HB2	1	0.19
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	13	0.19
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	5	0.19
(1,878)	1:56:A:CYS:HA	1:57:A:GLY:HA3	20	0.19
(1,849)	1:54:A:GLY:HA2	1:70:A:PRO:HD2	10	0.19
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	4	0.19
(1,761)	1:48:A:ASN:HA	1:49:A:PRO:HG3	11	0.19
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	4	0.19
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	6	0.19
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	14	0.19
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	15	0.19
(1,748)	1:47:A:PRO:HD2	1:47:A:PRO:HG3	20	0.19
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	10	0.19
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	13	0.19
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	16	0.19
(1,705)	1:44:A:ALA:HB1	1:65:A:TYR:HA	7	0.19
(1,699)	1:44:A:ALA:HB3	1:64:A:TYR:HB3	10	0.19
(1,695)	1:44:A:ALA:HB3	1:45:A:CYS:HB3	10	0.19
(1,688)	1:44:A:ALA:HA	1:36:A:THR:HG21	18	0.19
(1,685)	1:43:A:ASN:HA	1:35:A:TYR:H	1	0.19
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	13	0.19
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	10	0.19
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	7	0.19
(1,605)	1:37:A:GLY:H	1:36:A:THR:HG23	1	0.19
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	2	0.19
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	18	0.19
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	15	0.19
(1,489)	1:29:A:CYS:HA	1:18:A:THR:HG22	3	0.19
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	1	0.19
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	10	0.19
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	10	0.19
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	11	0.19
(1,395)	1:22:A:ARG:HG2	1:21:A:LYS:HA	6	0.19
(1,390)	1:22:A:ARG:HG3	1:22:A:ARG:HA	5	0.19
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	17	0.19
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	1	0.19
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	18	0.19
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	13	0.19
(1,342)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	6	0.19
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	15	0.19
(1,297)	1:18:A:THR:HB	1:30:A:TYR:HE1	1	0.19
(1,280)	1:32:A:ARG:H	1:17:A:GLY:HA3	20	0.19
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	1	0.19
(1,252)	1:16:A:GLY:H	1:14:A:ARG:HA	4	0.19
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	14	0.19
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	18	0.19
(1,230)	1:10:A:PRO:HG3	1:11:A:TYR:H	2	0.19
(1,199)	1:9:A:SER:H	1:9:A:SER:HB3	7	0.19
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	20	0.19
(1,150)	1:6:A:ASN:HA	1:21:A:LYS:HG3	20	0.19
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	16	0.19
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	3	0.19
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	6	0.19
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	9	0.19
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	11	0.19
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	12	0.19
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	5	0.19
(1,54)	1:60:A:TYR:HE1	1:60:A:TYR:HB3	8	0.19
(1,34)	1:64:A:TYR:H	1:63:A:PRO:HB3	11	0.19
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	7	0.18
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	16	0.18
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	2	0.18
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	4	0.18
(1,1877)	1:22:A:ARG:H	1:21:A:LYS:HB3	7	0.18
(1,1844)	1:78:A:CYS:H	1:74:A:TYR:HA	9	0.18
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	9	0.18
(1,1810)	1:73:A:TYR:H	1:81:A:LYS:HA	20	0.18
(1,1809)	1:73:A:TYR:H	1:72:A:GLY:HA3	15	0.18
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	14	0.18
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	4	0.18
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	7	0.18
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	11	0.18
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	18	0.18
(1,1773)	1:64:A:TYR:H	1:64:A:TYR:HD1	13	0.18
(1,1754)	1:59:A:VAL:H	1:58:A:TYR:HD1	14	0.18
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	14	0.18
(1,1713)	1:48:A:ASN:H	1:49:A:PRO:HD2	2	0.18
(1,1696)	1:44:A:ALA:H	1:43:A:ASN:HB2	4	0.18
(1,1683)	1:42:A:TYR:H	1:42:A:TYR:HB3	16	0.18
(1,1683)	1:42:A:TYR:H	1:42:A:TYR:HB3	20	0.18
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	12	0.18
(1,1658)	1:39:A:ASN:H	1:41:A:GLN:H	5	0.18
(1,1636)	1:34:A:GLY:H	1:35:A:TYR:HD1	20	0.18
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	19	0.18
(1,1579)	1:24:A:LEU:H	1:25:A:TYR:HA	4	0.18
(1,1579)	1:24:A:LEU:H	1:25:A:TYR:HA	5	0.18
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	3	0.18
(1,1539)	1:17:A:GLY:H	1:32:A:ARG:HG2	1	0.18
(1,1539)	1:17:A:GLY:H	1:32:A:ARG:HG2	6	0.18
(1,1512)	1:6:A:ASN:H	1:6:A:ASN:HB3	10	0.18
(1,1510)	1:6:A:ASN:H	1:5:A:PRO:HB2	20	0.18
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	14	0.18
(1,1491)	1:2:A:VAL:HA	1:3:A:TYR:HB2	16	0.18
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	14	0.18
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	16	0.18
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	16	0.18
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	19	0.18
(1,1444)	1:38:A:LYS:HD2	1:38:A:LYS:HB2	9	0.18
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	15	0.18
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	7	0.18
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	13	0.18
(1,1419)	1:60:A:TYR:HA	1:59:A:VAL:HG22	11	0.18
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	4	0.18
(1,1385)	1:83:A:TYR:HA	1:82:A:LYS:HD2	4	0.18
(1,1379)	1:82:A:LYS:HE2	1:74:A:TYR:HE1	9	0.18
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	7	0.18
(1,1337)	1:81:A:LYS:HB2	1:83:A:TYR:HE1	3	0.18
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	3	0.18
(1,1281)	1:79:A:GLN:HG2	1:80:A:LEU:HB2	10	0.18
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	2	0.18
(1,1220)	1:76:A:LYS:HA	1:76:A:LYS:HG2	12	0.18
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	14	0.18
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	7	0.18
(1,1191)	1:73:A:TYR:HB3	1:70:A:PRO:HD3	13	0.18
(1,1182)	1:72:A:GLY:HA2	1:71:A:TYR:HD1	19	0.18
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	1	0.18
(1,1147)	1:70:A:PRO:HD2	1:73:A:TYR:HD1	14	0.18
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	5	0.18
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	16	0.18
(1,1080)	1:68:A:SER:HB3	1:55:A:THR:HB	5	0.18
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	6	0.18
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	8	0.18
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	16	0.18
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	7	0.18
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	19	0.18
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	7	0.18
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	13	0.18
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	3	0.18
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	20	0.18
(1,994)	1:63:A:PRO:HA	1:63:A:PRO:HG3	8	0.18
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	2	0.18
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG11	10	0.18
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG11	18	0.18
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG11	16	0.18
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	19	0.18
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	3	0.18
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	18	0.18
(1,879)	1:56:A:CYS:HA	1:68:A:SER:HB2	12	0.18
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	2	0.18
(1,849)	1:54:A:GLY:HA2	1:70:A:PRO:HD2	9	0.18
(1,806)	1:51:A:LEU:HA	1:52:A:ASN:HB3	16	0.18
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	4	0.18
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	10	0.18
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	12	0.18
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	20	0.18
(1,695)	1:44:A:ALA:HB1	1:45:A:CYS:HB3	17	0.18
(1,683)	1:43:A:ASN:HA	1:44:A:ALA:HA	3	0.18
(1,639)	1:39:A:ASN:H	1:38:A:LYS:HG2	6	0.18
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	9	0.18
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	5	0.18
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	15	0.18
(1,551)	1:33:A:LYS:HB3	1:33:A:LYS:HE2	1	0.18
(1,549)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	1	0.18
(1,549)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	5	0.18
(1,549)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	15	0.18
(1,541)	1:33:A:LYS:HA	1:32:A:ARG:HB2	12	0.18
(1,531)	1:32:A:ARG:HD2	1:33:A:LYS:H	13	0.18
(1,488)	1:28:A:LYS:HE2	1:28:A:LYS:HA	7	0.18
(1,480)	1:28:A:LYS:HB2	1:22:A:ARG:H	3	0.18
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	14	0.18
(1,455)	1:27:A:TYR:HA	1:21:A:LYS:HB2	16	0.18
(1,455)	1:27:A:TYR:HA	1:21:A:LYS:HB2	18	0.18
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	20	0.18
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	12	0.18
(1,434)	1:26:A:SER:H	1:25:A:TYR:HB3	16	0.18
(1,419)	1:24:A:LEU:HA	1:25:A:TYR:HD1	11	0.18
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	9	0.18
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	20	0.18
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	18	0.18
(1,304)	1:18:A:THR:HG21	1:30:A:TYR:HB2	4	0.18
(1,257)	1:15:A:ASN:H	1:14:A:ARG:HG2	13	0.18
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	12	0.18
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	5	0.18
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	17	0.18
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	5	0.18
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	14	0.18
(1,181)	1:7:A:PRO:HG2	1:27:A:TYR:HA	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:8:A:CYS:H	1:7:A:PRO:HD2	9	0.18
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	2	0.18
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	19	0.18
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	14	0.18
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	15	0.18
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	18	0.18
(1,135)	1:5:A:PRO:HD3	1:5:A:PRO:HG2	20	0.18
(1,96)	1:3:A:TYR:HB2	1:3:A:TYR:H	7	0.18
(1,59)	1:71:A:TYR:HD1	1:71:A:TYR:HB2	3	0.18
(1,46)	1:11:A:TYR:HE1	1:11:A:TYR:HB3	11	0.18
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	8	0.18
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	14	0.18
(1,10)	1:31:A:CYS:HB2	1:32:A:ARG:HA	2	0.18
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	13	0.18
(1,6)	1:7:A:PRO:HD2	1:21:A:LYS:HE3	10	0.18
(1,5)	1:7:A:PRO:HD3	1:21:A:LYS:HE3	13	0.18
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	4	0.17
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	15	0.17
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	4	0.17
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	1	0.17
(1,1809)	1:73:A:TYR:H	1:72:A:GLY:HA3	9	0.17
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	12	0.17
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	15	0.17
(1,1755)	1:59:A:VAL:H	1:60:A:TYR:H	17	0.17
(1,1754)	1:59:A:VAL:H	1:58:A:TYR:HD1	6	0.17
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	15	0.17
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	16	0.17
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	20	0.17
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	12	0.17
(1,1709)	1:46:A:PHE:H	1:46:A:PHE:HD1	16	0.17
(1,1683)	1:42:A:TYR:H	1:42:A:TYR:HB3	3	0.17
(1,1683)	1:42:A:TYR:H	1:42:A:TYR:HB3	8	0.17
(1,1683)	1:42:A:TYR:H	1:42:A:TYR:HB3	15	0.17
(1,1676)	1:79:A:GLN:H	1:75:A:GLY:HA2	3	0.17
(1,1636)	1:34:A:GLY:H	1:35:A:TYR:HD1	8	0.17
(1,1635)	1:34:A:GLY:H	1:33:A:LYS:HB3	9	0.17
(1,1632)	1:33:A:LYS:H	1:32:A:ARG:HB3	12	0.17
(1,1571)	1:82:A:LYS:H	1:74:A:TYR:HD1	9	0.17
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	18	0.17
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	2	0.17
(1,1512)	1:6:A:ASN:H	1:6:A:ASN:HB3	17	0.17
(1,1486)	1:7:A:PRO:HD3	1:6:A:ASN:HB3	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	12	0.17
(1,1477)	1:18:A:THR:HG22	1:19:A:CYS:HB3	18	0.17
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	8	0.17
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	15	0.17
(1,1426)	1:53:A:GLY:HA2	1:52:A:ASN:H	12	0.17
(1,1417)	1:63:A:PRO:HB2	1:64:A:TYR:HD1	1	0.17
(1,1417)	1:63:A:PRO:HB2	1:64:A:TYR:HD1	10	0.17
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	5	0.17
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	7	0.17
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	20	0.17
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	11	0.17
(1,1337)	1:81:A:LYS:HB2	1:83:A:TYR:HE1	5	0.17
(1,1286)	1:79:A:GLN:HG2	1:78:A:CYS:H	17	0.17
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	18	0.17
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	11	0.17
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	16	0.17
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	14	0.17
(1,1241)	1:77:A:GLN:HG2	1:49:A:PRO:HG2	11	0.17
(1,1226)	1:76:A:LYS:HA	1:75:A:GLY:H	13	0.17
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	9	0.17
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	15	0.17
(1,1133)	1:71:A:TYR:H	1:70:A:PRO:HB2	7	0.17
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	19	0.17
(1,1122)	1:70:A:PRO:HB2	1:70:A:PRO:HD3	11	0.17
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	5	0.17
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	16	0.17
(1,1064)	1:66:A:LYS:HG3	1:59:A:VAL:HG21	2	0.17
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG11	4	0.17
(1,1053)	1:65:A:TYR:HB3	1:65:A:TYR:HD1	10	0.17
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	14	0.17
(1,1036)	1:59:A:VAL:HG11	1:65:A:TYR:HA	2	0.17
(1,979)	1:60:A:TYR:H	1:60:A:TYR:HB3	9	0.17
(1,960)	1:59:A:VAL:HG23	1:60:A:TYR:HB2	13	0.17
(1,956)	1:60:A:TYR:H	1:59:A:VAL:HG12	15	0.17
(1,931)	1:59:A:VAL:HB	1:66:A:LYS:HB3	20	0.17
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	2	0.17
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	9	0.17
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	13	0.17
(1,852)	1:54:A:GLY:HA2	1:53:A:GLY:H	15	0.17
(1,816)	1:51:A:LEU:HB3	1:52:A:ASN:HA	1	0.17
(1,792)	1:50:A:CYS:HA	1:77:A:GLN:HG3	7	0.17
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	2	0.17
(1,738)	1:47:A:PRO:HA	1:47:A:PRO:HB2	5	0.17
(1,705)	1:44:A:ALA:HB2	1:65:A:TYR:HA	9	0.17
(1,700)	1:44:A:ALA:HB1	1:64:A:TYR:HB2	20	0.17
(1,683)	1:43:A:ASN:HA	1:44:A:ALA:HA	12	0.17
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	20	0.17
(1,623)	1:38:A:LYS:HB3	1:38:A:LYS:HE2	12	0.17
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	5	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	1	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	3	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	4	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	7	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	8	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	12	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	14	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	15	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	16	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	17	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	19	0.17
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	20	0.17
(1,600)	1:36:A:THR:HG21	1:64:A:TYR:HB2	9	0.17
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	1	0.17
(1,588)	1:58:A:TYR:HB2	1:59:A:VAL:H	15	0.17
(1,586)	1:73:A:TYR:HA	1:74:A:TYR:HE1	1	0.17
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	2	0.17
(1,554)	1:33:A:LYS:HD3	1:33:A:LYS:HA	16	0.17
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	2	0.17
(1,516)	1:32:A:ARG:HA	1:35:A:TYR:HD1	16	0.17
(1,490)	1:29:A:CYS:HA	1:20:A:LYS:HG2	17	0.17
(1,480)	1:28:A:LYS:HB2	1:22:A:ARG:H	19	0.17
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	20	0.17
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	13	0.17
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	6	0.17
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	7	0.17
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	11	0.17
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	18	0.17
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	2	0.17
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	17	0.17
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	4	0.17
(1,396)	1:22:A:ARG:HG2	1:22:A:ARG:HA	15	0.17
(1,396)	1:22:A:ARG:HG2	1:22:A:ARG:HA	18	0.17
(1,392)	1:22:A:ARG:HG3	1:22:A:ARG:H	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:22:A:ARG:HG3	1:22:A:ARG:H	16	0.17
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	19	0.17
(1,343)	1:81:A:LYS:HE2	1:81:A:LYS:HG2	16	0.17
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	5	0.17
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	14	0.17
(1,318)	1:19:A:CYS:HB2	1:18:A:THR:HG23	17	0.17
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	15	0.17
(1,231)	1:10:A:PRO:HG2	1:11:A:TYR:H	9	0.17
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	7	0.17
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	20	0.17
(1,219)	1:11:A:TYR:H	1:10:A:PRO:HB2	14	0.17
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	17	0.17
(1,199)	1:9:A:SER:H	1:9:A:SER:HB3	1	0.17
(1,199)	1:9:A:SER:H	1:9:A:SER:HB3	5	0.17
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	9	0.17
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	12	0.17
(1,182)	1:7:A:PRO:HG2	1:27:A:TYR:HD1	18	0.17
(1,175)	1:8:A:CYS:H	1:7:A:PRO:HD2	1	0.17
(1,167)	1:7:A:PRO:HD3	1:21:A:LYS:HG2	18	0.17
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	14	0.17
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	18	0.17
(1,129)	1:5:A:PRO:HD2	1:4:A:TYR:H	1	0.17
(1,126)	1:5:A:PRO:HD2	1:4:A:TYR:HB3	10	0.17
(1,123)	1:5:A:PRO:HB3	1:3:A:TYR:HD1	19	0.17
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	2	0.17
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	10	0.17
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	18	0.17
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	7	0.17
(1,6)	1:7:A:PRO:HD2	1:21:A:LYS:HE3	6	0.17
(1,1869)	1:53:A:GLY:H	1:51:A:LEU:HD21	12	0.16
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	10	0.16
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	13	0.16
(1,1843)	1:78:A:CYS:H	1:77:A:GLN:HB2	18	0.16
(1,1836)	1:76:A:LYS:H	1:75:A:GLY:H	15	0.16
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	11	0.16
(1,1803)	1:72:A:GLY:H	1:73:A:TYR:HD1	11	0.16
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	20	0.16
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	5	0.16
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	14	0.16
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	16	0.16
(1,1752)	1:59:A:VAL:H	1:64:A:TYR:HB3	5	0.16
(1,1751)	1:59:A:VAL:H	1:66:A:LYS:HB2	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1740)	1:57:A:GLY:H	1:66:A:LYS:HB2	2	0.16
(1,1740)	1:57:A:GLY:H	1:66:A:LYS:HB2	7	0.16
(1,1713)	1:48:A:ASN:H	1:49:A:PRO:HD2	5	0.16
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	5	0.16
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	12	0.16
(1,1702)	1:45:A:CYS:H	1:58:A:TYR:HE1	10	0.16
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	2	0.16
(1,1676)	1:79:A:GLN:H	1:75:A:GLY:HA2	15	0.16
(1,1671)	1:41:A:GLN:H	1:39:A:ASN:HB3	5	0.16
(1,1646)	1:36:A:THR:H	1:44:A:ALA:HB3	13	0.16
(1,1635)	1:34:A:GLY:H	1:33:A:LYS:HB3	13	0.16
(1,1635)	1:34:A:GLY:H	1:33:A:LYS:HB3	18	0.16
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	10	0.16
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD13	12	0.16
(1,1572)	1:23:A:GLY:H	1:22:A:ARG:HB2	7	0.16
(1,1571)	1:82:A:LYS:H	1:74:A:TYR:HD1	18	0.16
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	5	0.16
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	20	0.16
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	11	0.16
(1,1512)	1:6:A:ASN:H	1:6:A:ASN:HB3	6	0.16
(1,1486)	1:7:A:PRO:HD3	1:6:A:ASN:HB3	1	0.16
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	6	0.16
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	16	0.16
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	20	0.16
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	8	0.16
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	19	0.16
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	2	0.16
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	15	0.16
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	14	0.16
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	4	0.16
(1,1426)	1:53:A:GLY:HA2	1:52:A:ASN:H	20	0.16
(1,1400)	1:76:A:LYS:HD2	1:76:A:LYS:HE2	3	0.16
(1,1400)	1:76:A:LYS:HD2	1:76:A:LYS:HE2	17	0.16
(1,1400)	1:76:A:LYS:HD2	1:76:A:LYS:HE2	18	0.16
(1,1400)	1:76:A:LYS:HD2	1:76:A:LYS:HE2	19	0.16
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	1	0.16
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	13	0.16
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	18	0.16
(1,1381)	1:82:A:LYS:HG2	1:74:A:TYR:HE1	19	0.16
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	17	0.16
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	10	0.16
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	12	0.16
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	16	0.16
(1,1347)	1:82:A:LYS:HA	1:82:A:LYS:HG2	7	0.16
(1,1338)	1:81:A:LYS:HB3	1:83:A:TYR:HE1	6	0.16
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	2	0.16
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	13	0.16
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	19	0.16
(1,1247)	1:77:A:GLN:HG2	1:78:A:CYS:H	16	0.16
(1,1228)	1:75:A:GLY:HA3	1:76:A:LYS:HG3	19	0.16
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	12	0.16
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	18	0.16
(1,1131)	1:70:A:PRO:HB3	1:73:A:TYR:HD1	15	0.16
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	4	0.16
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	10	0.16
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	2	0.16
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	13	0.16
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	11	0.16
(1,1054)	1:65:A:TYR:HB2	1:58:A:TYR:HD1	20	0.16
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	11	0.16
(1,1030)	1:64:A:TYR:HB3	1:65:A:TYR:HB3	9	0.16
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	11	0.16
(1,960)	1:59:A:VAL:HG21	1:60:A:TYR:HB2	18	0.16
(1,934)	1:59:A:VAL:HB	1:60:A:TYR:HD1	14	0.16
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	6	0.16
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	12	0.16
(1,849)	1:54:A:GLY:HA2	1:70:A:PRO:HD2	8	0.16
(1,816)	1:51:A:LEU:HB3	1:52:A:ASN:HA	19	0.16
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	10	0.16
(1,700)	1:44:A:ALA:HB1	1:64:A:TYR:HB2	3	0.16
(1,667)	1:40:A:CYS:HB3	1:39:A:ASN:HA	7	0.16
(1,634)	1:66:A:LYS:HE2	1:66:A:LYS:HG2	6	0.16
(1,633)	1:66:A:LYS:HE2	1:66:A:LYS:HG3	3	0.16
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	1	0.16
(1,623)	1:38:A:LYS:HB3	1:38:A:LYS:HE2	1	0.16
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	3	0.16
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	18	0.16
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	2	0.16
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	5	0.16
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	9	0.16
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	18	0.16
(1,597)	1:36:A:THR:HG23	1:42:A:TYR:HB3	8	0.16
(1,597)	1:36:A:THR:HG22	1:42:A:TYR:HB3	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:34:A:GLY:HA2	1:58:A:TYR:HE1	11	0.16
(1,565)	1:34:A:GLY:HA3	1:35:A:TYR:HD1	11	0.16
(1,538)	1:33:A:LYS:HA	1:33:A:LYS:HG2	6	0.16
(1,532)	1:32:A:ARG:HD2	1:32:A:ARG:H	12	0.16
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	1	0.16
(1,510)	1:31:A:CYS:HB2	1:40:A:CYS:HB2	12	0.16
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	9	0.16
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	10	0.16
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	14	0.16
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	20	0.16
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD22	13	0.16
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	10	0.16
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	11	0.16
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	12	0.16
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	5	0.16
(1,274)	1:17:A:GLY:HA2	1:32:A:ARG:H	15	0.16
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	2	0.16
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	14	0.16
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	17	0.16
(1,244)	1:13:A:CYS:HA	1:39:A:ASN:HB2	6	0.16
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	7	0.16
(1,230)	1:10:A:PRO:HG3	1:11:A:TYR:H	10	0.16
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	3	0.16
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	8	0.16
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	16	0.16
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	1	0.16
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	15	0.16
(1,176)	1:7:A:PRO:HG2	1:21:A:LYS:HG3	19	0.16
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	18	0.16
(1,141)	1:6:A:ASN:H	1:5:A:PRO:HG2	11	0.16
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	5	0.16
(1,134)	1:4:A:TYR:H	1:5:A:PRO:HD3	12	0.16
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	2	0.16
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	14	0.16
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	8	0.16
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	18	0.16
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	2	0.16
(1,62)	1:73:A:TYR:HD1	1:73:A:TYR:HA	3	0.16
(1,62)	1:73:A:TYR:HD1	1:73:A:TYR:HA	13	0.16
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	4	0.16
(1,10)	1:31:A:CYS:HB2	1:32:A:ARG:HA	5	0.16
(1,1892)	1:65:A:TYR:H	1:64:A:TYR:HB3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1886)	1:22:A:ARG:H	1:27:A:TYR:HD1	1	0.15
(1,1886)	1:22:A:ARG:H	1:27:A:TYR:HD1	8	0.15
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	1	0.15
(1,1826)	1:75:A:GLY:H	1:77:A:GLN:H	13	0.15
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	6	0.15
(1,1800)	1:72:A:GLY:H	1:82:A:LYS:HB3	18	0.15
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	8	0.15
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	12	0.15
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	20	0.15
(1,1755)	1:59:A:VAL:H	1:60:A:TYR:H	8	0.15
(1,1755)	1:59:A:VAL:H	1:60:A:TYR:H	11	0.15
(1,1751)	1:59:A:VAL:H	1:66:A:LYS:HB2	9	0.15
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	7	0.15
(1,1740)	1:57:A:GLY:H	1:66:A:LYS:HB2	8	0.15
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	10	0.15
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	1	0.15
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	6	0.15
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	20	0.15
(1,1619)	1:31:A:CYS:H	1:30:A:TYR:HB2	8	0.15
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	12	0.15
(1,1583)	1:25:A:TYR:H	1:24:A:LEU:HD21	6	0.15
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	1	0.15
(1,1539)	1:17:A:GLY:H	1:32:A:ARG:HG2	3	0.15
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	12	0.15
(1,1486)	1:7:A:PRO:HD3	1:6:A:ASN:HB3	12	0.15
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	5	0.15
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	2	0.15
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	4	0.15
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	6	0.15
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	20	0.15
(1,1400)	1:76:A:LYS:HD2	1:76:A:LYS:HE2	1	0.15
(1,1400)	1:76:A:LYS:HD2	1:76:A:LYS:HE2	5	0.15
(1,1400)	1:76:A:LYS:HD2	1:76:A:LYS:HE2	7	0.15
(1,1400)	1:76:A:LYS:HD2	1:76:A:LYS:HE2	9	0.15
(1,1400)	1:76:A:LYS:HD2	1:76:A:LYS:HE2	15	0.15
(1,1400)	1:76:A:LYS:HD2	1:76:A:LYS:HE2	20	0.15
(1,1393)	1:83:A:TYR:HB2	1:83:A:TYR:HE1	16	0.15
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	12	0.15
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	10	0.15
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	11	0.15
(1,1337)	1:81:A:LYS:HB2	1:83:A:TYR:HE1	19	0.15
(1,1281)	1:79:A:GLN:HG2	1:80:A:LEU:HB2	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	3	0.15
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	9	0.15
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	11	0.15
(1,1249)	1:77:A:GLN:HG2	1:51:A:LEU:H	6	0.15
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	3	0.15
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	6	0.15
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	14	0.15
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	20	0.15
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	9	0.15
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	3	0.15
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	13	0.15
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	10	0.15
(1,1109)	1:69:A:CYS:HB3	1:73:A:TYR:H	2	0.15
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	1	0.15
(1,1078)	1:57:A:GLY:H	1:67:A:CYS:HA	5	0.15
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	13	0.15
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	16	0.15
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	5	0.15
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	8	0.15
(1,1050)	1:65:A:TYR:HB3	1:58:A:TYR:HA	19	0.15
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	3	0.15
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG13	9	0.15
(1,960)	1:59:A:VAL:HG21	1:60:A:TYR:HB2	4	0.15
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	12	0.15
(1,907)	1:58:A:TYR:HA	1:64:A:TYR:HB2	6	0.15
(1,881)	1:56:A:CYS:HA	1:67:A:CYS:HA	18	0.15
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	3	0.15
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	20	0.15
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	1	0.15
(1,818)	1:51:A:LEU:H	1:51:A:LEU:HB3	2	0.15
(1,818)	1:51:A:LEU:H	1:51:A:LEU:HB3	7	0.15
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	14	0.15
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	5	0.15
(1,707)	1:44:A:ALA:HB3	1:58:A:TYR:HD1	18	0.15
(1,705)	1:44:A:ALA:HB2	1:65:A:TYR:HA	4	0.15
(1,703)	1:44:A:ALA:HB3	1:58:A:TYR:HA	20	0.15
(1,688)	1:44:A:ALA:HA	1:36:A:THR:HG23	2	0.15
(1,637)	1:38:A:LYS:HG3	1:38:A:LYS:H	13	0.15
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	12	0.15
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	10	0.15
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	1	0.15
(1,588)	1:58:A:TYR:HB2	1:59:A:VAL:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:73:A:TYR:HA	1:81:A:LYS:HG2	4	0.15
(1,534)	1:32:A:ARG:HG2	1:32:A:ARG:HB2	9	0.15
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	6	0.15
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	19	0.15
(1,447)	1:26:A:SER:HA	1:27:A:TYR:HD1	13	0.15
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	8	0.15
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	17	0.15
(1,440)	1:43:A:ASN:HB2	1:46:A:PHE:H	18	0.15
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	18	0.15
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	15	0.15
(1,396)	1:22:A:ARG:HG2	1:22:A:ARG:HA	19	0.15
(1,391)	1:22:A:ARG:HG3	1:27:A:TYR:HA	20	0.15
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	5	0.15
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	15	0.15
(1,349)	1:20:A:LYS:HG2	1:30:A:TYR:HE1	12	0.15
(1,304)	1:18:A:THR:HG21	1:30:A:TYR:HB2	19	0.15
(1,297)	1:18:A:THR:HB	1:30:A:TYR:HE1	19	0.15
(1,278)	1:17:A:GLY:HA3	1:31:A:CYS:HA	12	0.15
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	11	0.15
(1,239)	1:13:A:CYS:HA	1:14:A:ARG:HG2	10	0.15
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	1	0.15
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	5	0.15
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	9	0.15
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	12	0.15
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	14	0.15
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	15	0.15
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	16	0.15
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	17	0.15
(1,227)	1:10:A:PRO:HG3	1:10:A:PRO:HD2	18	0.15
(1,222)	1:70:A:PRO:HD3	1:73:A:TYR:HD1	6	0.15
(1,219)	1:11:A:TYR:H	1:10:A:PRO:HB2	5	0.15
(1,212)	1:10:A:PRO:HA	1:9:A:SER:H	4	0.15
(1,196)	1:9:A:SER:HB3	1:8:A:CYS:HA	15	0.15
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	8	0.15
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	8	0.15
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	1	0.15
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	17	0.15
(1,59)	1:71:A:TYR:HD1	1:71:A:TYR:HB2	19	0.15
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	7	0.15
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	11	0.15
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	15	0.15
(1,38)	1:82:A:LYS:H	1:74:A:TYR:HE1	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:31:A:CYS:HB2	1:32:A:ARG:HA	18	0.15
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	10	0.15
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	15	0.15
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	19	0.15
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	20	0.15
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	5	0.14
(1,1874)	1:34:A:GLY:H	1:33:A:LYS:HB2	7	0.14
(1,1868)	1:53:A:GLY:H	1:51:A:LEU:HA	6	0.14
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	1	0.14
(1,1843)	1:78:A:CYS:H	1:77:A:GLN:HB2	1	0.14
(1,1843)	1:78:A:CYS:H	1:77:A:GLN:HB2	5	0.14
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	3	0.14
(1,1824)	1:74:A:TYR:H	1:80:A:LEU:H	20	0.14
(1,1810)	1:73:A:TYR:H	1:81:A:LYS:HA	13	0.14
(1,1809)	1:73:A:TYR:H	1:72:A:GLY:HA3	18	0.14
(1,1776)	1:65:A:TYR:H	1:59:A:VAL:HB	15	0.14
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	15	0.14
(1,1754)	1:59:A:VAL:H	1:58:A:TYR:HD1	3	0.14
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	2	0.14
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	18	0.14
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	2	0.14
(1,1711)	1:48:A:ASN:H	1:47:A:PRO:HB3	7	0.14
(1,1709)	1:46:A:PHE:H	1:46:A:PHE:HD1	5	0.14
(1,1696)	1:44:A:ALA:H	1:43:A:ASN:HB2	13	0.14
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	3	0.14
(1,1514)	1:6:A:ASN:H	1:7:A:PRO:HD2	16	0.14
(1,1513)	1:6:A:ASN:H	1:7:A:PRO:HD3	11	0.14
(1,1513)	1:6:A:ASN:H	1:7:A:PRO:HD3	14	0.14
(1,1510)	1:6:A:ASN:H	1:5:A:PRO:HB2	5	0.14
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	13	0.14
(1,1484)	1:11:A:TYR:HB2	1:11:A:TYR:HD1	10	0.14
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	7	0.14
(1,1477)	1:18:A:THR:HG23	1:19:A:CYS:HB3	15	0.14
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	6	0.14
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	18	0.14
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	1	0.14
(1,1470)	1:21:A:LYS:HD3	1:21:A:LYS:HA	17	0.14
(1,1463)	1:24:A:LEU:HA	1:25:A:TYR:HB3	3	0.14
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	17	0.14
(1,1432)	1:47:A:PRO:HG3	1:48:A:ASN:H	4	0.14
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	9	0.14
(1,1426)	1:53:A:GLY:HA2	1:52:A:ASN:H	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	14	0.14
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	10	0.14
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	16	0.14
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	14	0.14
(1,1228)	1:75:A:GLY:HA3	1:76:A:LYS:HG3	16	0.14
(1,1226)	1:76:A:LYS:HA	1:75:A:GLY:H	2	0.14
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	11	0.14
(1,1220)	1:76:A:LYS:HA	1:76:A:LYS:HG2	4	0.14
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	9	0.14
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	11	0.14
(1,1191)	1:73:A:TYR:HB3	1:70:A:PRO:HD3	5	0.14
(1,1146)	1:70:A:PRO:HD2	1:73:A:TYR:HA	3	0.14
(1,1122)	1:70:A:PRO:HB2	1:70:A:PRO:HD3	3	0.14
(1,1122)	1:70:A:PRO:HB2	1:70:A:PRO:HD3	4	0.14
(1,1108)	1:69:A:CYS:HB2	1:73:A:TYR:H	14	0.14
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	10	0.14
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	4	0.14
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	3	0.14
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	2	0.14
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	15	0.14
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	16	0.14
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	19	0.14
(1,1047)	1:58:A:TYR:H	1:65:A:TYR:HA	20	0.14
(1,971)	1:61:A:GLY:H	1:60:A:TYR:HA	17	0.14
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG13	15	0.14
(1,936)	1:77:A:GLN:HG3	1:78:A:CYS:H	8	0.14
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	16	0.14
(1,906)	1:58:A:TYR:HA	1:65:A:TYR:HB2	12	0.14
(1,875)	1:68:A:SER:H	1:55:A:THR:HG22	3	0.14
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	16	0.14
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	19	0.14
(1,804)	1:51:A:LEU:H	1:50:A:CYS:HB3	8	0.14
(1,704)	1:44:A:ALA:HB3	1:35:A:TYR:HA	14	0.14
(1,699)	1:44:A:ALA:HB2	1:64:A:TYR:HB3	19	0.14
(1,683)	1:43:A:ASN:HA	1:44:A:ALA:HA	18	0.14
(1,664)	1:40:A:CYS:HB2	1:31:A:CYS:HA	9	0.14
(1,631)	1:38:A:LYS:HD2	1:38:A:LYS:H	11	0.14
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	14	0.14
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	15	0.14
(1,617)	1:38:A:LYS:HA	1:38:A:LYS:HE3	17	0.14
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	6	0.14
(1,616)	1:38:A:LYS:HA	1:38:A:LYS:HB2	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:38:A:LYS:HA	1:38:A:LYS:HG2	3	0.14
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	4	0.14
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	17	0.14
(1,548)	1:33:A:LYS:HB2	1:33:A:LYS:HE3	13	0.14
(1,536)	1:32:A:ARG:HG2	1:35:A:TYR:HD1	8	0.14
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	6	0.14
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	11	0.14
(1,493)	1:29:A:CYS:HA	1:30:A:TYR:HD1	7	0.14
(1,479)	1:28:A:LYS:HB2	1:21:A:LYS:HA	7	0.14
(1,478)	1:66:A:LYS:HB2	1:66:A:LYS:HE2	9	0.14
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	9	0.14
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	10	0.14
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	15	0.14
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	1	0.14
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	2	0.14
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	16	0.14
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	13	0.14
(1,392)	1:22:A:ARG:HG3	1:22:A:ARG:H	2	0.14
(1,391)	1:22:A:ARG:HG3	1:27:A:TYR:HA	2	0.14
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	2	0.14
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	3	0.14
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	7	0.14
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	15	0.14
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	14	0.14
(1,359)	1:21:A:LYS:HA	1:27:A:TYR:HD1	9	0.14
(1,352)	1:21:A:LYS:HA	1:21:A:LYS:HG3	16	0.14
(1,345)	1:82:A:LYS:H	1:81:A:LYS:HE2	6	0.14
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	4	0.14
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	6	0.14
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	1	0.14
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	3	0.14
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	4	0.14
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	8	0.14
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	10	0.14
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	11	0.14
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	12	0.14
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	17	0.14
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	18	0.14
(1,315)	1:19:A:CYS:HB3	1:11:A:TYR:HD1	5	0.14
(1,292)	1:18:A:THR:HB	1:30:A:TYR:HB3	12	0.14
(1,286)	1:18:A:THR:HA	1:30:A:TYR:HD1	18	0.14
(1,265)	1:15:A:ASN:HB2	1:35:A:TYR:HD1	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:15:A:ASN:HB2	1:35:A:TYR:HD1	12	0.14
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	2	0.14
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	1	0.14
(1,96)	1:3:A:TYR:HB2	1:3:A:TYR:H	15	0.14
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	4	0.14
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	20	0.14
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	3	0.14
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	19	0.14
(1,7)	1:28:A:LYS:HA	1:27:A:TYR:HA	8	0.14
(2,12)	1:55:A:THR:N	1:68:A:SER:O	9	0.13
(2,12)	1:55:A:THR:N	1:68:A:SER:O	13	0.13
(1,1886)	1:22:A:ARG:H	1:27:A:TYR:HD1	12	0.13
(1,1874)	1:34:A:GLY:H	1:33:A:LYS:HB2	8	0.13
(1,1874)	1:34:A:GLY:H	1:33:A:LYS:HB2	11	0.13
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	12	0.13
(1,1843)	1:78:A:CYS:H	1:77:A:GLN:HB2	2	0.13
(1,1826)	1:75:A:GLY:H	1:77:A:GLN:H	9	0.13
(1,1826)	1:75:A:GLY:H	1:77:A:GLN:H	20	0.13
(1,1810)	1:73:A:TYR:H	1:81:A:LYS:HA	16	0.13
(1,1800)	1:72:A:GLY:H	1:82:A:LYS:HB3	9	0.13
(1,1777)	1:65:A:TYR:H	1:65:A:TYR:HB2	10	0.13
(1,1777)	1:65:A:TYR:H	1:65:A:TYR:HB2	19	0.13
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	8	0.13
(1,1755)	1:59:A:VAL:H	1:60:A:TYR:H	2	0.13
(1,1755)	1:59:A:VAL:H	1:60:A:TYR:H	5	0.13
(1,1755)	1:59:A:VAL:H	1:60:A:TYR:H	13	0.13
(1,1755)	1:59:A:VAL:H	1:60:A:TYR:H	15	0.13
(1,1741)	1:57:A:GLY:H	1:56:A:CYS:HB2	5	0.13
(1,1719)	1:51:A:LEU:H	1:52:A:ASN:HB3	11	0.13
(1,1714)	1:50:A:CYS:H	1:49:A:PRO:HG2	2	0.13
(1,1709)	1:46:A:PHE:H	1:46:A:PHE:HD1	3	0.13
(1,1683)	1:42:A:TYR:H	1:42:A:TYR:HB3	4	0.13
(1,1683)	1:42:A:TYR:H	1:42:A:TYR:HB3	13	0.13
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	19	0.13
(1,1673)	1:41:A:GLN:H	1:42:A:TYR:HB2	1	0.13
(1,1635)	1:34:A:GLY:H	1:33:A:LYS:HB3	5	0.13
(1,1580)	1:24:A:LEU:H	1:25:A:TYR:HD1	13	0.13
(1,1579)	1:24:A:LEU:H	1:25:A:TYR:HA	6	0.13
(1,1546)	1:17:A:GLY:H	1:31:A:CYS:HA	10	0.13
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	3	0.13
(1,1483)	1:14:A:ARG:HA	1:14:A:ARG:HG2	14	0.13
(1,1442)	1:39:A:ASN:H	1:38:A:LYS:HB3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	5	0.13
(1,1426)	1:53:A:GLY:HA2	1:52:A:ASN:H	6	0.13
(1,1413)	1:28:A:LYS:HA	1:28:A:LYS:HB2	2	0.13
(1,1401)	1:76:A:LYS:HA	1:76:A:LYS:HE2	7	0.13
(1,1379)	1:82:A:LYS:HE2	1:74:A:TYR:HE1	12	0.13
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	4	0.13
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	18	0.13
(1,1360)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	12	0.13
(1,1319)	1:79:A:GLN:HG3	1:80:A:LEU:HD23	18	0.13
(1,1275)	1:79:A:GLN:HB3	1:80:A:LEU:HG	9	0.13
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	4	0.13
(1,1270)	1:79:A:GLN:HA	1:79:A:GLN:HG2	17	0.13
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	10	0.13
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	15	0.13
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	20	0.13
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	1	0.13
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	2	0.13
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	20	0.13
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	13	0.13
(1,1159)	1:70:A:PRO:HG3	1:55:A:THR:H	5	0.13
(1,1157)	1:70:A:PRO:HG2	1:73:A:TYR:HD1	17	0.13
(1,1150)	1:70:A:PRO:HD2	1:71:A:TYR:H	3	0.13
(1,1149)	1:70:A:PRO:HD2	1:72:A:GLY:H	6	0.13
(1,1133)	1:71:A:TYR:H	1:70:A:PRO:HB2	2	0.13
(1,1087)	1:69:A:CYS:H	1:68:A:SER:HB2	8	0.13
(1,1071)	1:67:A:CYS:HA	1:50:A:CYS:HB3	13	0.13
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	5	0.13
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	12	0.13
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	1	0.13
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	13	0.13
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	17	0.13
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	1	0.13
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	3	0.13
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	8	0.13
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	15	0.13
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	17	0.13
(1,950)	1:58:A:TYR:HA	1:59:A:VAL:HG11	2	0.13
(1,947)	1:61:A:GLY:HA2	1:59:A:VAL:HG12	15	0.13
(1,909)	1:58:A:TYR:HA	1:58:A:TYR:HE1	5	0.13
(1,849)	1:54:A:GLY:HA2	1:70:A:PRO:HD2	14	0.13
(1,816)	1:51:A:LEU:HB3	1:52:A:ASN:HA	9	0.13
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,768)	1:48:A:ASN:HA	1:50:A:CYS:H	8	0.13
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	3	0.13
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	16	0.13
(1,717)	1:45:A:CYS:HA	1:58:A:TYR:HE1	20	0.13
(1,707)	1:44:A:ALA:HB3	1:58:A:TYR:HD1	12	0.13
(1,705)	1:44:A:ALA:HB2	1:65:A:TYR:HA	18	0.13
(1,683)	1:43:A:ASN:HA	1:44:A:ALA:HA	9	0.13
(1,683)	1:43:A:ASN:HA	1:44:A:ALA:HA	10	0.13
(1,683)	1:43:A:ASN:HA	1:44:A:ALA:HA	17	0.13
(1,683)	1:43:A:ASN:HA	1:44:A:ALA:HA	20	0.13
(1,681)	1:43:A:ASN:HA	1:42:A:TYR:HB3	17	0.13
(1,656)	1:40:A:CYS:HB3	1:32:A:ARG:HG2	3	0.13
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	13	0.13
(1,597)	1:36:A:THR:HG21	1:42:A:TYR:HB3	1	0.13
(1,592)	1:36:A:THR:HB	1:44:A:ALA:HB1	18	0.13
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	12	0.13
(1,510)	1:31:A:CYS:HB2	1:40:A:CYS:HB2	15	0.13
(1,491)	1:29:A:CYS:HA	1:13:A:CYS:HB2	3	0.13
(1,489)	1:29:A:CYS:HA	1:18:A:THR:HG23	13	0.13
(1,485)	1:66:A:LYS:HB3	1:65:A:TYR:HA	3	0.13
(1,485)	1:66:A:LYS:HB3	1:65:A:TYR:HA	16	0.13
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	4	0.13
(1,454)	1:27:A:TYR:HA	1:28:A:LYS:HB2	7	0.13
(1,426)	1:24:A:LEU:HB2	1:25:A:TYR:HB2	11	0.13
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	4	0.13
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	7	0.13
(1,413)	1:24:A:LEU:HA	1:24:A:LEU:HB3	3	0.13
(1,393)	1:22:A:ARG:HG3	1:28:A:LYS:H	20	0.13
(1,385)	1:22:A:ARG:HB3	1:22:A:ARG:H	5	0.13
(1,372)	1:21:A:LYS:HG3	1:21:A:LYS:H	16	0.13
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	9	0.13
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	20	0.13
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	1	0.13
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	5	0.13
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	10	0.13
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	3	0.13
(1,330)	1:20:A:LYS:HB2	1:20:A:LYS:HD3	7	0.13
(1,330)	1:20:A:LYS:HB2	1:20:A:LYS:HD3	14	0.13
(1,328)	1:20:A:LYS:HB3	1:30:A:TYR:HD1	19	0.13
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	2	0.13
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	5	0.13
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	7	0.13
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	9	0.13
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	13	0.13
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	14	0.13
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	15	0.13
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	16	0.13
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	19	0.13
(1,323)	1:20:A:LYS:HB3	1:20:A:LYS:HG2	20	0.13
(1,286)	1:18:A:THR:HA	1:30:A:TYR:HD1	13	0.13
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	9	0.13
(1,253)	1:15:A:ASN:H	1:14:A:ARG:HB2	4	0.13
(1,245)	1:13:A:CYS:HA	1:39:A:ASN:HA	13	0.13
(1,245)	1:13:A:CYS:HA	1:39:A:ASN:HA	16	0.13
(1,243)	1:13:A:CYS:HA	1:14:A:ARG:HD2	16	0.13
(1,230)	1:10:A:PRO:HG3	1:11:A:TYR:H	6	0.13
(1,212)	1:10:A:PRO:HA	1:9:A:SER:H	3	0.13
(1,199)	1:9:A:SER:H	1:9:A:SER:HB3	12	0.13
(1,194)	1:8:A:CYS:HB2	1:7:A:PRO:HA	20	0.13
(1,182)	1:7:A:PRO:HG2	1:27:A:TYR:HD1	17	0.13
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	10	0.13
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	12	0.13
(1,62)	1:73:A:TYR:HD1	1:73:A:TYR:HA	6	0.13
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	2	0.13
(1,12)	1:34:A:GLY:HA3	1:58:A:TYR:HB3	15	0.13
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	6	0.13
(1,7)	1:28:A:LYS:HA	1:27:A:TYR:HA	11	0.13
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	12	0.13
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	18	0.13
(1,1888)	1:82:A:LYS:H	1:83:A:TYR:HE1	10	0.12
(1,1874)	1:34:A:GLY:H	1:33:A:LYS:HB2	9	0.12
(1,1874)	1:34:A:GLY:H	1:33:A:LYS:HB2	12	0.12
(1,1867)	1:59:A:VAL:H	1:64:A:TYR:HB2	12	0.12
(1,1860)	1:83:A:TYR:H	1:74:A:TYR:HD1	20	0.12
(1,1844)	1:78:A:CYS:H	1:74:A:TYR:HA	20	0.12
(1,1809)	1:73:A:TYR:H	1:72:A:GLY:HA3	2	0.12
(1,1809)	1:73:A:TYR:H	1:72:A:GLY:HA3	16	0.12
(1,1809)	1:73:A:TYR:H	1:72:A:GLY:HA3	20	0.12
(1,1800)	1:72:A:GLY:H	1:82:A:LYS:HB3	16	0.12
(1,1781)	1:66:A:LYS:H	1:66:A:LYS:HG2	13	0.12
(1,1777)	1:65:A:TYR:H	1:65:A:TYR:HB2	1	0.12
(1,1777)	1:65:A:TYR:H	1:65:A:TYR:HB2	8	0.12
(1,1777)	1:65:A:TYR:H	1:65:A:TYR:HB2	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1776)	1:65:A:TYR:H	1:59:A:VAL:HB	5	0.12
(1,1755)	1:59:A:VAL:H	1:60:A:TYR:H	3	0.12
(1,1754)	1:59:A:VAL:H	1:58:A:TYR:HD1	12	0.12
(1,1750)	1:58:A:TYR:H	1:59:A:VAL:H	5	0.12
(1,1745)	1:57:A:GLY:H	1:65:A:TYR:HD1	4	0.12
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	2	0.12
(1,1732)	1:54:A:GLY:H	1:55:A:THR:H	4	0.12
(1,1716)	1:50:A:CYS:H	1:49:A:PRO:HD3	8	0.12
(1,1709)	1:46:A:PHE:H	1:46:A:PHE:HD1	2	0.12
(1,1703)	1:45:A:CYS:H	1:58:A:TYR:HD1	19	0.12
(1,1683)	1:42:A:TYR:H	1:42:A:TYR:HB3	11	0.12
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	15	0.12
(1,1656)	1:39:A:ASN:H	1:37:A:GLY:HA2	12	0.12
(1,1656)	1:39:A:ASN:H	1:37:A:GLY:HA2	14	0.12
(1,1640)	1:35:A:TYR:H	1:36:A:THR:HA	3	0.12
(1,1636)	1:34:A:GLY:H	1:35:A:TYR:HD1	6	0.12
(1,1635)	1:34:A:GLY:H	1:33:A:LYS:HB3	1	0.12
(1,1635)	1:34:A:GLY:H	1:33:A:LYS:HB3	4	0.12
(1,1631)	1:32:A:ARG:H	1:35:A:TYR:H	6	0.12
(1,1603)	1:29:A:CYS:H	1:28:A:LYS:HE3	16	0.12
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	5	0.12
(1,1588)	1:26:A:SER:H	1:24:A:LEU:HB3	9	0.12
(1,1579)	1:24:A:LEU:H	1:25:A:TYR:HA	1	0.12
(1,1579)	1:24:A:LEU:H	1:25:A:TYR:HA	19	0.12
(1,1571)	1:82:A:LYS:H	1:74:A:TYR:HD1	6	0.12
(1,1547)	1:17:A:GLY:H	1:14:A:ARG:H	17	0.12
(1,1534)	1:15:A:ASN:H	1:16:A:GLY:HA3	7	0.12
(1,1512)	1:6:A:ASN:H	1:6:A:ASN:HB3	8	0.12
(1,1511)	1:6:A:ASN:H	1:6:A:ASN:HB2	4	0.12
(1,1492)	1:2:A:VAL:HG12	1:3:A:TYR:H	17	0.12
(1,1477)	1:18:A:THR:HG23	1:19:A:CYS:HB3	12	0.12
(1,1477)	1:18:A:THR:HG22	1:19:A:CYS:HB3	14	0.12
(1,1477)	1:18:A:THR:HG23	1:19:A:CYS:HB3	17	0.12
(1,1450)	1:33:A:LYS:HA	1:33:A:LYS:HE3	9	0.12
(1,1419)	1:60:A:TYR:HA	1:59:A:VAL:HG23	15	0.12
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	6	0.12
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	18	0.12
(1,1383)	1:82:A:LYS:H	1:82:A:LYS:HG2	6	0.12
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	1	0.12
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	13	0.12
(1,1373)	1:72:A:GLY:HA2	1:82:A:LYS:HD2	15	0.12
(1,1365)	1:82:A:LYS:HB3	1:74:A:TYR:HE1	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	5	0.12
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	7	0.12
(1,1361)	1:82:A:LYS:HB2	1:81:A:LYS:HA	19	0.12
(1,1221)	1:76:A:LYS:HA	1:76:A:LYS:HG3	5	0.12
(1,1220)	1:76:A:LYS:HA	1:76:A:LYS:HG2	1	0.12
(1,1209)	1:75:A:GLY:HA2	1:79:A:GLN:HG3	18	0.12
(1,1205)	1:75:A:GLY:HA3	1:80:A:LEU:HB3	8	0.12
(1,1176)	1:72:A:GLY:HA3	1:82:A:LYS:HB3	8	0.12
(1,1175)	1:72:A:GLY:HA2	1:82:A:LYS:HB3	6	0.12
(1,1159)	1:70:A:PRO:HG3	1:55:A:THR:H	1	0.12
(1,1133)	1:71:A:TYR:H	1:70:A:PRO:HB2	1	0.12
(1,1124)	1:70:A:PRO:HD3	1:70:A:PRO:HB3	11	0.12
(1,1095)	1:55:A:THR:H	1:69:A:CYS:HA	17	0.12
(1,1094)	1:54:A:GLY:H	1:69:A:CYS:HA	13	0.12
(1,1075)	1:55:A:THR:HB	1:67:A:CYS:HA	15	0.12
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	14	0.12
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	4	0.12
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	7	0.12
(1,1009)	1:63:A:PRO:HD2	1:63:A:PRO:HA	15	0.12
(1,1009)	1:63:A:PRO:HD2	1:63:A:PRO:HA	18	0.12
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	2	0.12
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	4	0.12
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	7	0.12
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	11	0.12
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	12	0.12
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	13	0.12
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	18	0.12
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	19	0.12
(1,966)	1:60:A:TYR:HA	1:59:A:VAL:HG12	13	0.12
(1,960)	1:59:A:VAL:HG22	1:60:A:TYR:HB2	19	0.12
(1,946)	1:59:A:VAL:HG13	1:61:A:GLY:HA3	9	0.12
(1,940)	1:59:A:VAL:HG12	1:66:A:LYS:HG2	14	0.12
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	8	0.12
(1,849)	1:54:A:GLY:HA2	1:70:A:PRO:HD2	16	0.12
(1,846)	1:54:A:GLY:HA3	1:70:A:PRO:HG2	17	0.12
(1,838)	1:53:A:GLY:HA2	1:70:A:PRO:HG3	3	0.12
(1,771)	1:49:A:PRO:HA	1:49:A:PRO:HG3	4	0.12
(1,771)	1:49:A:PRO:HA	1:49:A:PRO:HG3	6	0.12
(1,771)	1:49:A:PRO:HA	1:49:A:PRO:HG3	7	0.12
(1,771)	1:49:A:PRO:HA	1:49:A:PRO:HG3	11	0.12
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	15	0.12
(1,759)	1:46:A:PHE:HA	1:47:A:PRO:HG3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:44:A:ALA:HB1	1:34:A:GLY:HA2	16	0.12
(1,633)	1:66:A:LYS:HE2	1:66:A:LYS:HG3	12	0.12
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	2	0.12
(1,617)	1:38:A:LYS:HA	1:38:A:LYS:HE3	15	0.12
(1,597)	1:36:A:THR:HG22	1:42:A:TYR:HB3	16	0.12
(1,592)	1:36:A:THR:HB	1:44:A:ALA:HB2	17	0.12
(1,522)	1:32:A:ARG:HB3	1:35:A:TYR:HD1	4	0.12
(1,516)	1:32:A:ARG:HA	1:35:A:TYR:HD1	19	0.12
(1,509)	1:31:A:CYS:H	1:31:A:CYS:HB3	5	0.12
(1,489)	1:29:A:CYS:HA	1:18:A:THR:HG23	12	0.12
(1,478)	1:66:A:LYS:HB2	1:66:A:LYS:HE2	15	0.12
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	6	0.12
(1,458)	1:27:A:TYR:HA	1:27:A:TYR:HD1	18	0.12
(1,455)	1:27:A:TYR:HA	1:21:A:LYS:HB2	5	0.12
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	5	0.12
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	19	0.12
(1,404)	1:23:A:GLY:HA3	1:22:A:ARG:HA	8	0.12
(1,396)	1:22:A:ARG:HG2	1:22:A:ARG:HA	4	0.12
(1,393)	1:22:A:ARG:HG3	1:28:A:LYS:H	9	0.12
(1,377)	1:22:A:ARG:HA	1:27:A:TYR:HA	11	0.12
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	2	0.12
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	3	0.12
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	11	0.12
(1,315)	1:19:A:CYS:HB3	1:11:A:TYR:HD1	4	0.12
(1,252)	1:16:A:GLY:H	1:14:A:ARG:HA	17	0.12
(1,248)	1:13:A:CYS:HB2	1:39:A:ASN:HA	1	0.12
(1,237)	1:11:A:TYR:HB3	1:11:A:TYR:H	11	0.12
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	7	0.12
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	9	0.12
(1,161)	1:7:A:PRO:HB3	1:21:A:LYS:HG3	4	0.12
(1,146)	1:6:A:ASN:HA	1:7:A:PRO:HD3	5	0.12
(1,143)	1:6:A:ASN:HA	1:7:A:PRO:HG3	19	0.12
(1,127)	1:5:A:PRO:HD2	1:5:A:PRO:HA	1	0.12
(1,124)	1:6:A:ASN:H	1:5:A:PRO:HB3	20	0.12
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	4	0.12
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	15	0.12
(1,79)	1:21:A:LYS:HB2	1:22:A:ARG:H	15	0.12
(1,57)	1:64:A:TYR:HE1	1:63:A:PRO:HA	5	0.12
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	20	0.12
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	2	0.12
(1,7)	1:28:A:LYS:HA	1:27:A:TYR:HA	14	0.12
(1,7)	1:28:A:LYS:HA	1:27:A:TYR:HA	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:55:A:THR:N	1:68:A:SER:O	3	0.11
(2,12)	1:55:A:THR:N	1:68:A:SER:O	17	0.11
(2,10)	1:18:A:THR:N	1:30:A:TYR:O	6	0.11
(2,8)	1:30:A:TYR:N	1:18:A:THR:O	17	0.11
(2,6)	1:28:A:LYS:N	1:20:A:LYS:O	16	0.11
(1,1894)	1:57:A:GLY:H	1:58:A:TYR:H	9	0.11
(1,1874)	1:34:A:GLY:H	1:33:A:LYS:HB2	1	0.11
(1,1874)	1:34:A:GLY:H	1:33:A:LYS:HB2	2	0.11
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	17	0.11
(1,1863)	1:68:A:SER:H	1:67:A:CYS:HB3	20	0.11
(1,1826)	1:75:A:GLY:H	1:77:A:GLN:H	2	0.11
(1,1821)	1:74:A:TYR:H	1:74:A:TYR:HE1	16	0.11
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	1	0.11
(1,1810)	1:73:A:TYR:H	1:81:A:LYS:HA	7	0.11
(1,1810)	1:73:A:TYR:H	1:81:A:LYS:HA	8	0.11
(1,1801)	1:72:A:GLY:H	1:71:A:TYR:HB3	5	0.11
(1,1783)	1:66:A:LYS:H	1:65:A:TYR:HD1	6	0.11
(1,1777)	1:65:A:TYR:H	1:65:A:TYR:HB2	15	0.11
(1,1777)	1:65:A:TYR:H	1:65:A:TYR:HB2	17	0.11
(1,1776)	1:65:A:TYR:H	1:59:A:VAL:HB	8	0.11
(1,1761)	1:61:A:GLY:H	1:60:A:TYR:HB3	12	0.11
(1,1754)	1:59:A:VAL:H	1:58:A:TYR:HD1	8	0.11
(1,1716)	1:50:A:CYS:H	1:49:A:PRO:HD3	1	0.11
(1,1713)	1:48:A:ASN:H	1:49:A:PRO:HD2	19	0.11
(1,1703)	1:45:A:CYS:H	1:58:A:TYR:HD1	5	0.11
(1,1703)	1:45:A:CYS:H	1:58:A:TYR:HD1	20	0.11
(1,1677)	1:41:A:GLN:H	1:42:A:TYR:HA	9	0.11
(1,1564)	1:20:A:LYS:H	1:27:A:TYR:HB3	9	0.11
(1,1512)	1:6:A:ASN:H	1:6:A:ASN:HB3	1	0.11
(1,1509)	1:3:A:TYR:H	1:4:A:TYR:H	15	0.11
(1,1493)	1:2:A:VAL:HG12	1:4:A:TYR:HD1	17	0.11
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	4	0.11
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	17	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	1	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	2	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	5	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	6	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	7	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	8	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	10	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	13	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	16	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	17	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	18	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	19	0.11
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	20	0.11
(1,1426)	1:53:A:GLY:HA2	1:52:A:ASN:H	4	0.11
(1,1426)	1:53:A:GLY:HA2	1:52:A:ASN:H	9	0.11
(1,1426)	1:53:A:GLY:HA2	1:52:A:ASN:H	10	0.11
(1,1419)	1:60:A:TYR:HA	1:59:A:VAL:HG22	8	0.11
(1,1419)	1:60:A:TYR:HA	1:59:A:VAL:HG23	13	0.11
(1,1419)	1:60:A:TYR:HA	1:59:A:VAL:HG22	16	0.11
(1,1419)	1:60:A:TYR:HA	1:59:A:VAL:HG22	17	0.11
(1,1417)	1:63:A:PRO:HB2	1:64:A:TYR:HD1	9	0.11
(1,1405)	1:73:A:TYR:HA	1:82:A:LYS:HG2	16	0.11
(1,1397)	1:79:A:GLN:HA	1:80:A:LEU:HG	20	0.11
(1,1380)	1:82:A:LYS:HB3	1:82:A:LYS:HG2	13	0.11
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	9	0.11
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	14	0.11
(1,1378)	1:82:A:LYS:HD2	1:82:A:LYS:HE2	18	0.11
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	12	0.11
(1,1285)	1:79:A:GLN:HG2	1:80:A:LEU:HA	4	0.11
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	10	0.11
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	20	0.11
(1,1248)	1:77:A:GLN:H	1:77:A:GLN:HG2	7	0.11
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	8	0.11
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	12	0.11
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	19	0.11
(1,1159)	1:70:A:PRO:HG3	1:55:A:THR:H	14	0.11
(1,1133)	1:71:A:TYR:H	1:70:A:PRO:HB2	9	0.11
(1,1133)	1:71:A:TYR:H	1:70:A:PRO:HB2	10	0.11
(1,1099)	1:69:A:CYS:HB2	1:70:A:PRO:HD3	18	0.11
(1,1077)	1:55:A:THR:H	1:67:A:CYS:HA	1	0.11
(1,1062)	1:66:A:LYS:HE2	1:59:A:VAL:HG12	2	0.11
(1,1051)	1:65:A:TYR:HB2	1:65:A:TYR:HE1	10	0.11
(1,1046)	1:59:A:VAL:H	1:65:A:TYR:HA	19	0.11
(1,1030)	1:64:A:TYR:HB3	1:65:A:TYR:HB3	18	0.11
(1,988)	1:62:A:TYR:HA	1:62:A:TYR:HD1	19	0.11
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	5	0.11
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	6	0.11
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	10	0.11
(1,961)	1:59:A:VAL:HA	1:59:A:VAL:HG22	20	0.11
(1,960)	1:59:A:VAL:HG22	1:60:A:TYR:HB2	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:57:A:GLY:HA2	1:66:A:LYS:HB2	17	0.11
(1,875)	1:68:A:SER:H	1:55:A:THR:HG21	19	0.11
(1,874)	1:56:A:CYS:H	1:55:A:THR:HG21	19	0.11
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	7	0.11
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	11	0.11
(1,859)	1:54:A:GLY:HA2	1:55:A:THR:HB	19	0.11
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	2	0.11
(1,800)	1:51:A:LEU:H	1:50:A:CYS:HA	14	0.11
(1,771)	1:49:A:PRO:HA	1:49:A:PRO:HG3	9	0.11
(1,771)	1:49:A:PRO:HA	1:49:A:PRO:HG3	14	0.11
(1,768)	1:48:A:ASN:HA	1:50:A:CYS:H	12	0.11
(1,767)	1:48:A:ASN:HA	1:46:A:PHE:HZ	17	0.11
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	20	0.11
(1,683)	1:43:A:ASN:HA	1:44:A:ALA:HA	19	0.11
(1,664)	1:40:A:CYS:HB2	1:31:A:CYS:HA	4	0.11
(1,641)	1:39:A:ASN:HA	1:29:A:CYS:HB3	18	0.11
(1,641)	1:39:A:ASN:HA	1:29:A:CYS:HB3	20	0.11
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	9	0.11
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	10	0.11
(1,609)	1:37:A:GLY:HA3	1:38:A:LYS:HG2	20	0.11
(1,603)	1:36:A:THR:HG23	1:42:A:TYR:HA	8	0.11
(1,603)	1:36:A:THR:HG23	1:42:A:TYR:HA	17	0.11
(1,597)	1:36:A:THR:HG21	1:42:A:TYR:HB3	17	0.11
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	8	0.11
(1,565)	1:34:A:GLY:HA3	1:35:A:TYR:HD1	5	0.11
(1,513)	1:31:A:CYS:HB2	1:35:A:TYR:HD1	13	0.11
(1,490)	1:29:A:CYS:HA	1:20:A:LYS:HG2	10	0.11
(1,489)	1:29:A:CYS:HA	1:18:A:THR:HG21	9	0.11
(1,485)	1:66:A:LYS:HB3	1:65:A:TYR:HA	7	0.11
(1,455)	1:27:A:TYR:HA	1:21:A:LYS:HB2	3	0.11
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	4	0.11
(1,441)	1:25:A:TYR:H	1:25:A:TYR:HB2	15	0.11
(1,418)	1:41:A:GLN:HA	1:40:A:CYS:HB2	2	0.11
(1,404)	1:23:A:GLY:HA3	1:22:A:ARG:HA	6	0.11
(1,404)	1:23:A:GLY:HA3	1:22:A:ARG:HA	11	0.11
(1,392)	1:22:A:ARG:HG3	1:22:A:ARG:H	4	0.11
(1,385)	1:22:A:ARG:HB3	1:22:A:ARG:H	4	0.11
(1,369)	1:21:A:LYS:HG3	1:21:A:LYS:HE3	12	0.11
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	17	0.11
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	6	0.11
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	9	0.11
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:20:A:LYS:HD2	1:21:A:LYS:H	12	0.11
(1,330)	1:20:A:LYS:HB2	1:20:A:LYS:HD3	8	0.11
(1,330)	1:20:A:LYS:HB2	1:20:A:LYS:HD3	13	0.11
(1,330)	1:20:A:LYS:HB2	1:20:A:LYS:HD3	20	0.11
(1,266)	1:15:A:ASN:HB2	1:14:A:ARG:H	10	0.11
(1,265)	1:15:A:ASN:HB2	1:35:A:TYR:HD1	15	0.11
(1,264)	1:15:A:ASN:HB2	1:35:A:TYR:HE1	5	0.11
(1,256)	1:14:A:ARG:HD2	1:14:A:ARG:H	10	0.11
(1,223)	1:70:A:PRO:HD3	1:55:A:THR:H	9	0.11
(1,203)	1:26:A:SER:HB2	1:27:A:TYR:HA	18	0.11
(1,183)	1:7:A:PRO:HG3	1:21:A:LYS:HG3	18	0.11
(1,181)	1:7:A:PRO:HG2	1:27:A:TYR:HA	4	0.11
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	19	0.11
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	10	0.11
(1,127)	1:5:A:PRO:HD2	1:5:A:PRO:HA	10	0.11
(1,127)	1:5:A:PRO:HD2	1:5:A:PRO:HA	19	0.11
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	7	0.11
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	11	0.11
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	19	0.11
(1,96)	1:3:A:TYR:HB2	1:3:A:TYR:H	6	0.11
(1,96)	1:3:A:TYR:HB2	1:3:A:TYR:H	11	0.11
(1,76)	1:21:A:LYS:HB3	1:21:A:LYS:HD3	3	0.11
(1,62)	1:73:A:TYR:HD1	1:73:A:TYR:HA	8	0.11
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	17	0.11
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	18	0.11
(1,7)	1:28:A:LYS:HA	1:27:A:TYR:HA	1	0.11
(1,7)	1:28:A:LYS:HA	1:27:A:TYR:HA	3	0.11
(1,7)	1:28:A:LYS:HA	1:27:A:TYR:HA	4	0.11
(1,7)	1:28:A:LYS:HA	1:29:A:CYS:HA	9	0.11
(1,7)	1:28:A:LYS:HA	1:27:A:TYR:HA	17	0.11
(2,12)	1:55:A:THR:N	1:68:A:SER:O	12	0.1
(2,12)	1:55:A:THR:N	1:68:A:SER:O	19	0.1
(1,1879)	1:22:A:ARG:H	1:23:A:GLY:HA2	4	0.1
(1,1874)	1:34:A:GLY:H	1:33:A:LYS:HB2	18	0.1
(1,1847)	1:78:A:CYS:H	1:80:A:LEU:H	2	0.1
(1,1843)	1:78:A:CYS:H	1:77:A:GLN:HB2	11	0.1
(1,1821)	1:74:A:TYR:H	1:74:A:TYR:HE1	8	0.1
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	17	0.1
(1,1813)	1:73:A:TYR:H	1:71:A:TYR:HD1	20	0.1
(1,1795)	1:69:A:CYS:H	1:70:A:PRO:HD3	3	0.1
(1,1764)	1:61:A:GLY:H	1:60:A:TYR:HD1	6	0.1
(1,1752)	1:59:A:VAL:H	1:64:A:TYR:HB3	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1743)	1:57:A:GLY:H	1:65:A:TYR:HA	3	0.1
(1,1671)	1:41:A:GLN:H	1:39:A:ASN:HB3	2	0.1
(1,1599)	1:28:A:LYS:H	1:20:A:LYS:HB3	14	0.1
(1,1571)	1:82:A:LYS:H	1:74:A:TYR:HD1	17	0.1
(1,1496)	1:43:A:ASN:HB3	1:42:A:TYR:HA	4	0.1
(1,1475)	1:20:A:LYS:HE3	1:20:A:LYS:HG2	7	0.1
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	4	0.1
(1,1474)	1:20:A:LYS:HE2	1:20:A:LYS:HD2	12	0.1
(1,1429)	1:52:A:ASN:H	1:51:A:LEU:HG	19	0.1
(1,1367)	1:82:A:LYS:HB3	1:74:A:TYR:HD1	3	0.1
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	13	0.1
(1,1359)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	20	0.1
(1,1353)	1:82:A:LYS:HA	1:74:A:TYR:HD1	7	0.1
(1,1266)	1:78:A:CYS:HB2	1:77:A:GLN:H	15	0.1
(1,1257)	1:69:A:CYS:HB3	1:78:A:CYS:HB2	7	0.1
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	5	0.1
(1,1197)	1:74:A:TYR:HB3	1:74:A:TYR:HE1	14	0.1
(1,1173)	1:72:A:GLY:HA2	1:82:A:LYS:HG2	18	0.1
(1,1159)	1:70:A:PRO:HG3	1:55:A:THR:H	18	0.1
(1,1131)	1:70:A:PRO:HB3	1:73:A:TYR:HD1	13	0.1
(1,1122)	1:70:A:PRO:HB2	1:70:A:PRO:HD3	6	0.1
(1,1070)	1:67:A:CYS:HA	1:66:A:LYS:HB3	14	0.1
(1,1058)	1:81:A:LYS:HA	1:81:A:LYS:HG2	6	0.1
(1,967)	1:60:A:TYR:HA	1:60:A:TYR:HB2	20	0.1
(1,961)	1:59:A:VAL:HA	1:59:A:VAL:HG22	6	0.1
(1,961)	1:59:A:VAL:HA	1:59:A:VAL:HG23	9	0.1
(1,958)	1:66:A:LYS:H	1:59:A:VAL:HG13	8	0.1
(1,958)	1:66:A:LYS:H	1:59:A:VAL:HG12	17	0.1
(1,957)	1:64:A:TYR:H	1:59:A:VAL:HG13	9	0.1
(1,885)	1:56:A:CYS:HB3	1:57:A:GLY:H	14	0.1
(1,850)	1:54:A:GLY:HA2	1:69:A:CYS:HA	1	0.1
(1,850)	1:54:A:GLY:HA2	1:69:A:CYS:HA	11	0.1
(1,773)	1:49:A:PRO:HA	1:49:A:PRO:HD2	2	0.1
(1,771)	1:49:A:PRO:HA	1:49:A:PRO:HG3	16	0.1
(1,771)	1:49:A:PRO:HA	1:49:A:PRO:HG3	17	0.1
(1,762)	1:48:A:ASN:HA	1:49:A:PRO:HB3	1	0.1
(1,760)	1:48:A:ASN:HA	1:49:A:PRO:HG2	18	0.1
(1,705)	1:44:A:ALA:HB3	1:65:A:TYR:HA	16	0.1
(1,704)	1:44:A:ALA:HB1	1:35:A:TYR:HA	8	0.1
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	4	0.1
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	6	0.1
(1,618)	1:38:A:LYS:HA	1:37:A:GLY:HA2	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:38:A:LYS:HA	1:38:A:LYS:HG2	15	0.1
(1,606)	1:44:A:ALA:H	1:36:A:THR:HG23	2	0.1
(1,596)	1:36:A:THR:HB	1:38:A:LYS:H	19	0.1
(1,509)	1:31:A:CYS:H	1:31:A:CYS:HB3	2	0.1
(1,509)	1:31:A:CYS:H	1:31:A:CYS:HB3	18	0.1
(1,404)	1:23:A:GLY:HA3	1:22:A:ARG:HA	1	0.1
(1,402)	1:23:A:GLY:HA2	1:24:A:LEU:HD22	15	0.1
(1,401)	1:23:A:GLY:HA3	1:24:A:LEU:HD22	3	0.1
(1,385)	1:22:A:ARG:HB3	1:22:A:ARG:H	18	0.1
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	10	0.1
(1,364)	1:21:A:LYS:HD3	1:21:A:LYS:H	12	0.1
(1,353)	1:21:A:LYS:HA	1:21:A:LYS:HG2	4	0.1
(1,304)	1:18:A:THR:HG21	1:30:A:TYR:HB2	5	0.1
(1,252)	1:16:A:GLY:H	1:14:A:ARG:HA	13	0.1
(1,207)	1:27:A:TYR:H	1:26:A:SER:HB2	20	0.1
(1,205)	1:26:A:SER:H	1:26:A:SER:HB2	20	0.1
(1,169)	1:7:A:PRO:HD3	1:6:A:ASN:HB2	12	0.1
(1,157)	1:7:A:PRO:HA	1:7:A:PRO:HD2	16	0.1
(1,137)	1:70:A:PRO:HG3	1:69:A:CYS:HA	9	0.1
(1,127)	1:5:A:PRO:HD2	1:5:A:PRO:HA	13	0.1
(1,127)	1:5:A:PRO:HD2	1:5:A:PRO:HA	17	0.1
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	2	0.1
(1,102)	1:4:A:TYR:HB2	1:4:A:TYR:HE1	3	0.1
(1,57)	1:64:A:TYR:HE1	1:63:A:PRO:HA	6	0.1
(1,46)	1:11:A:TYR:HE1	1:11:A:TYR:HB3	20	0.1
(1,43)	1:2:A:VAL:HG22	1:4:A:TYR:HD1	5	0.1
(1,42)	1:4:A:TYR:HD1	1:4:A:TYR:HB3	1	0.1
(1,35)	1:80:A:LEU:H	1:79:A:GLN:HB2	7	0.1

10 Dihedral-angle violation analysis [i](#)

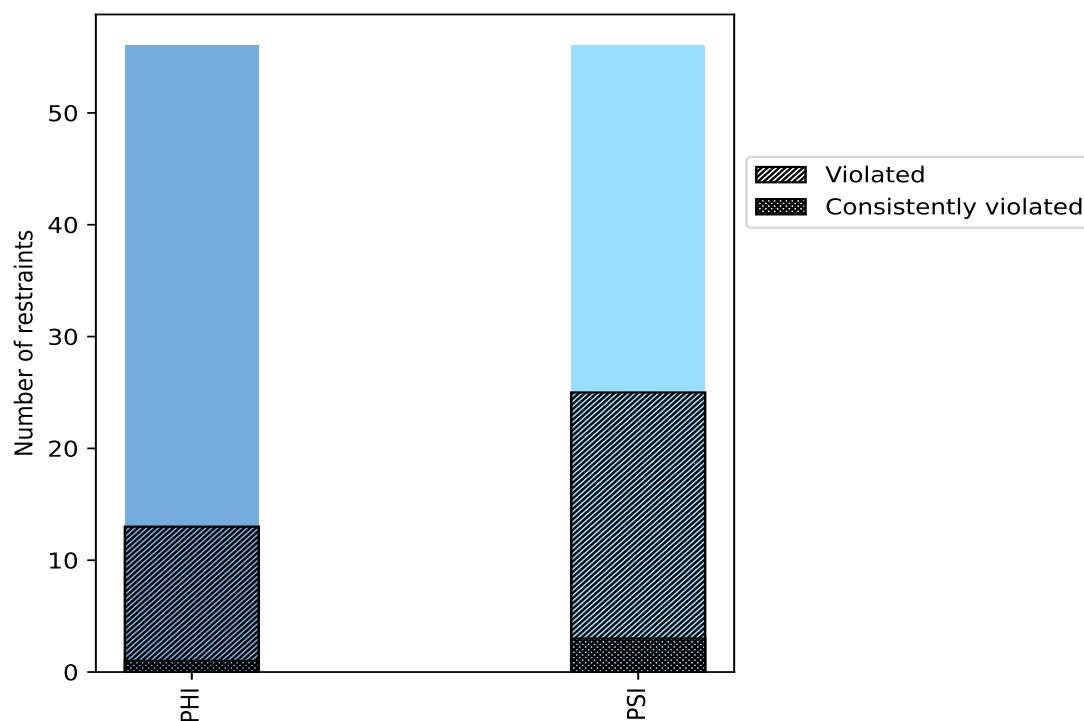
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	56	50.0	13	23.2	11.6	1	1.8	0.9
PSI	56	50.0	25	44.6	22.3	3	5.4	2.7
Total	112	100.0	38	33.9	33.9	4	3.6	3.6

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



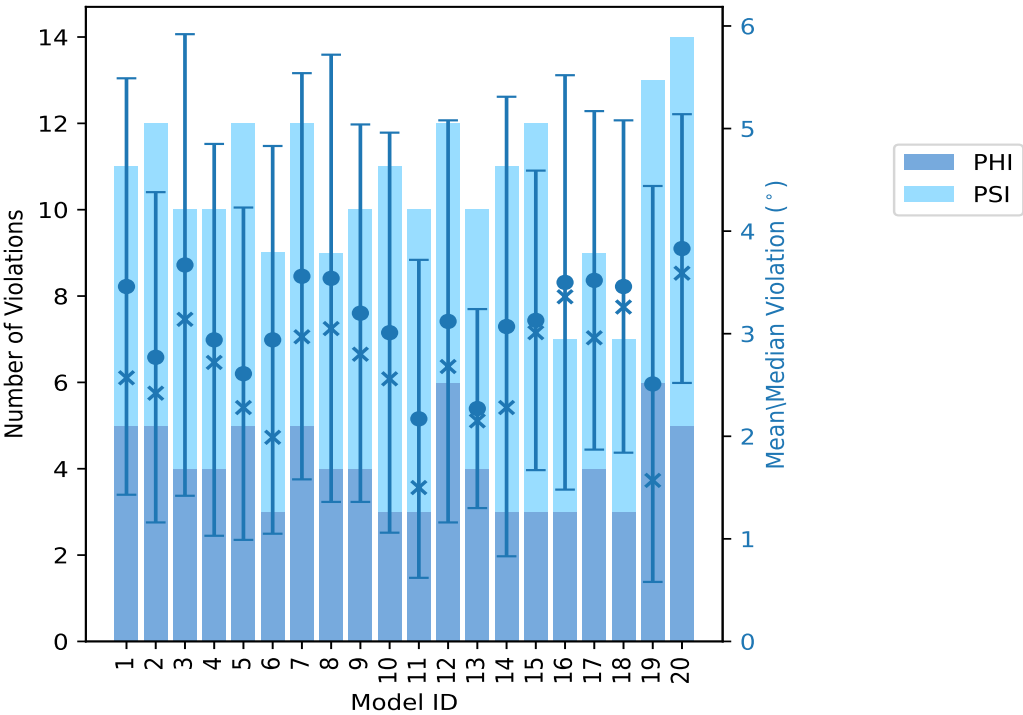
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	5	6	11	3.46	6.74	2.03	2.57
2	5	7	12	2.77	6.77	1.61	2.42
3	4	6	10	3.67	8.13	2.25	3.14
4	4	6	10	2.94	7.77	1.91	2.72
5	5	7	12	2.61	6.9	1.62	2.28
6	3	6	9	2.94	6.07	1.89	1.99
7	5	7	12	3.56	8.29	1.98	2.97
8	4	5	9	3.54	8.63	2.18	3.05
9	4	6	10	3.2	6.05	1.84	2.8
10	3	8	11	3.01	7.82	1.95	2.56
11	3	7	10	2.17	6.0	1.55	1.5
12	6	6	12	3.12	6.37	1.96	2.68
13	4	6	10	2.27	4.3	0.97	2.15
14	3	8	11	3.07	8.61	2.24	2.28
15	3	9	12	3.13	5.36	1.46	3.01
16	3	4	7	3.5	7.34	2.02	3.36
17	4	5	9	3.52	6.56	1.65	2.96
18	3	4	7	3.46	6.47	1.62	3.26
19	6	7	13	2.51	7.26	1.93	1.57
20	5	9	14	3.83	6.61	1.31	3.59

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
4	8	12	1	5.0
2	4	6	2	10.0
1	2	3	3	15.0
1	3	4	4	20.0
0	1	1	5	25.0
1	2	3	6	30.0
0	1	1	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
1	0	1	10	50.0
0	1	1	11	55.0

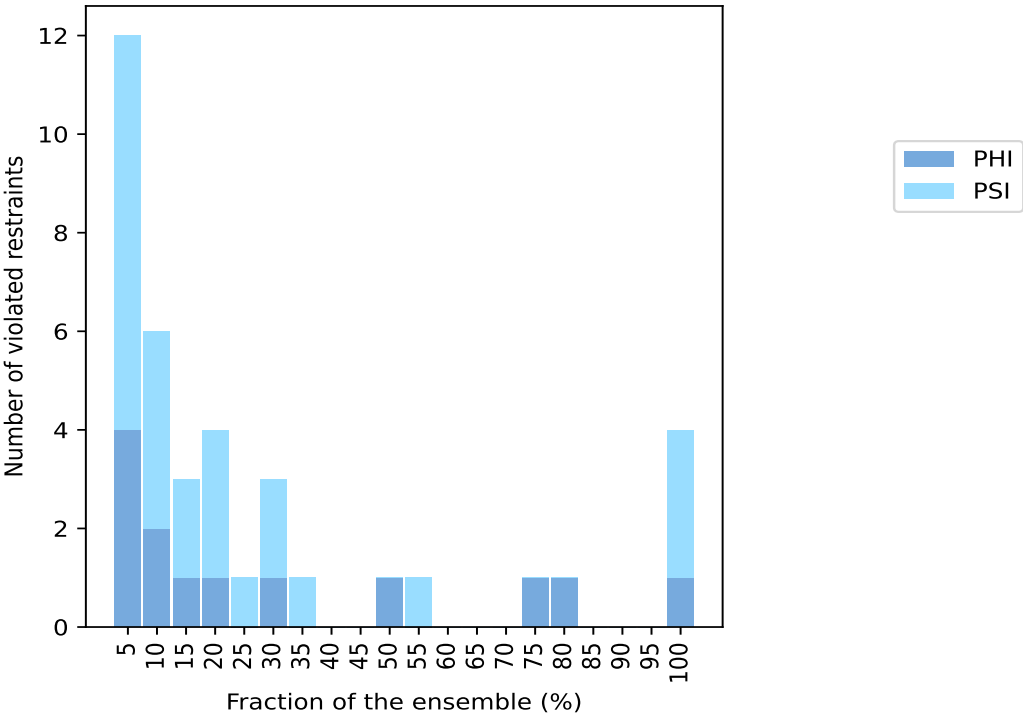
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
1	0	1	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
1	3	4	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

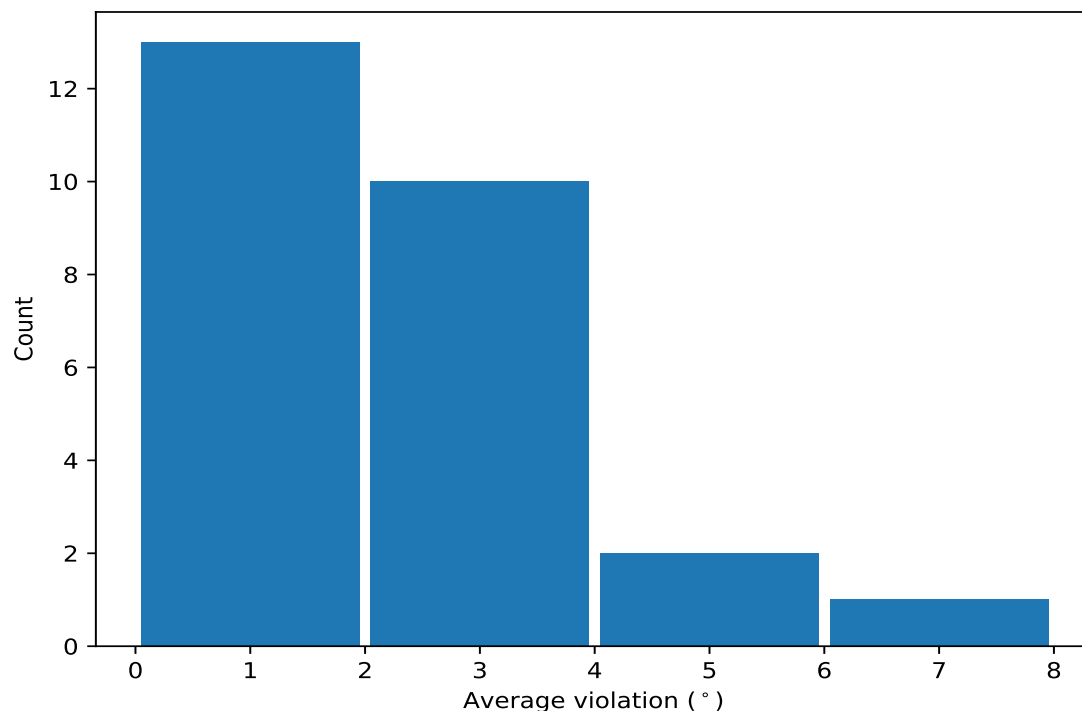


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	20	6.81	1.15	6.66
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	20	4.49	1.11	4.72
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	20	4.06	0.94	4.1
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	20	3.92	1.63	3.34
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	16	2.93	1.31	2.78
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	15	1.61	0.76	1.33
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	11	2.73	0.59	2.56
(1,33)	1:26:A:SER:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	10	2.78	0.87	2.93
(1,32)	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	1:27:A:TYR:N	7	2.62	1.13	2.52
(1,30)	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	1:26:A:SER:N	6	2.04	0.78	2.18
(1,105)	1:76:A:LYS:C	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	6	1.72	0.25	1.8
(1,14)	1:15:A:ASN:N	1:15:A:ASN:CA	1:15:A:ASN:C	1:16:A:GLY:N	6	1.66	0.43	1.54
(1,28)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:TYR:N	5	2.46	1.18	1.87
(1,80)	1:62:A:TYR:N	1:62:A:TYR:CA	1:62:A:TYR:C	1:63:A:PRO:N	4	1.68	0.35	1.63
(1,40)	1:30:A:TYR:N	1:30:A:TYR:CA	1:30:A:TYR:C	1:31:A:CYS:N	4	1.3	0.17	1.39
(1,43)	1:33:A:LYS:C	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	4	1.21	0.06	1.23
(1,58)	1:45:A:CYS:N	1:45:A:CYS:CA	1:45:A:CYS:C	1:46:A:PHE:N	4	1.2	0.17	1.16
(1,8)	1:10:A:PRO:N	1:10:A:PRO:CA	1:10:A:PRO:C	1:11:A:TYR:N	3	2.78	1.19	2.53
(1,50)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:ASN:N	3	1.69	0.4	1.86
(1,45)	1:35:A:TYR:C	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	3	1.12	0.1	1.08

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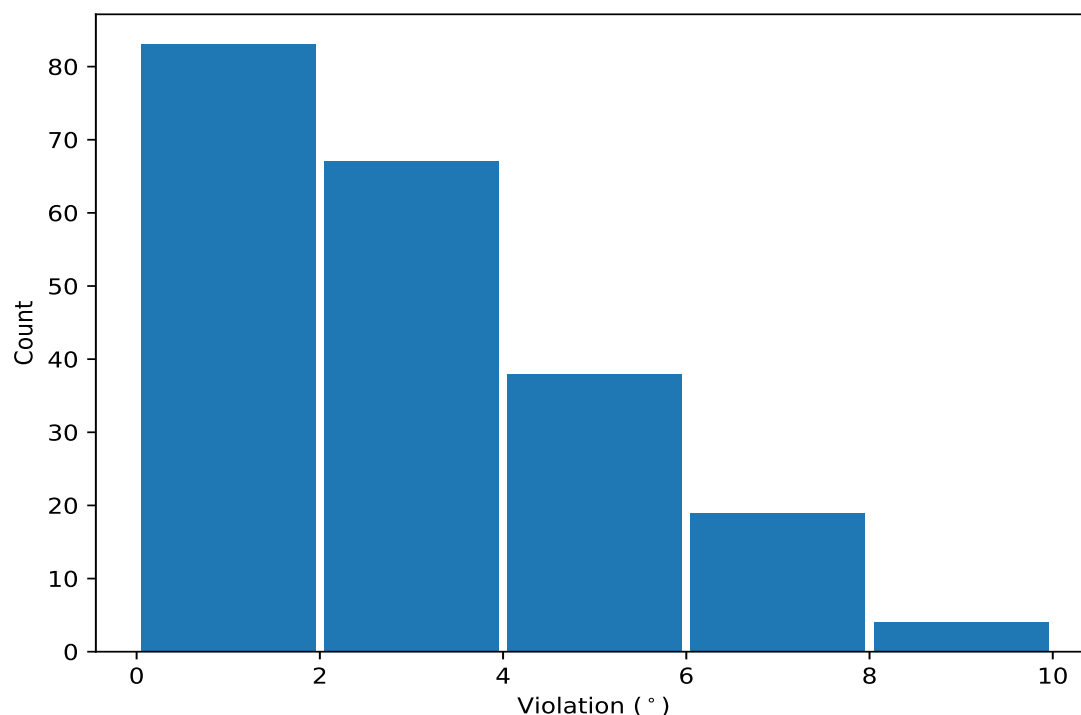
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,9)	1:10:A:PRO:C	1:11:A:TYR:N	1:11:A:TYR:CA	1:11:A:TYR:C	2	2.06	0.5	2.06
(1,68)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:ASN:N	2	2.01	0.99	2.01
(1,22)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:LYS:N	2	1.52	0.15	1.52
(1,38)	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	1:30:A:TYR:N	2	1.44	0.22	1.44
(1,20)	1:19:A:CYS:N	1:19:A:CYS:CA	1:19:A:CYS:C	1:20:A:LYS:N	2	1.29	0.03	1.29
(1,103)	1:75:A:GLY:C	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	2	1.18	0.18	1.18

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	8	8.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	14	8.61
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	7	8.29
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	3	8.13
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	10	7.82
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	4	7.77
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	16	7.34
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	19	7.26
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	5	6.9
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	2	6.77
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	1	6.74
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	20	6.61
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	3	6.59
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	17	6.56
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	18	6.47
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	12	6.37
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	14	6.36
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	1	6.19
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	7	6.18
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	12	6.1
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	6	6.07
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	9	6.05
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	11	6.0
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	6	5.77
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	19	5.42
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	20	5.41
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	15	5.36
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	9	5.35
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	2	5.3
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	7	5.28
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	17	5.27
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	20	5.23
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	1	5.18
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	1	5.17
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	8	5.11
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	17	5.05
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	15	5.04
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	9	4.98
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	16	4.9
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	18	4.82
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	19	4.82
(1,32)	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	1:27:A:TYR:N	20	4.8
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	12	4.77
(1,28)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:TYR:N	15	4.74
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	10	4.73
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	3	4.7
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	3	4.7
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	15	4.7
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	12	4.65
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	1	4.62
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	9	4.61
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	4	4.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,8)	1:10:A:PRO:N	1:10:A:PRO:CA	1:10:A:PRO:C	1:11:A:TYR:N	20	4.35
(1,101)	1:74:A:TYR:C	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	13	4.3
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	10	4.29
(1,33)	1:26:A:SER:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	20	4.25
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	11	4.21
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	8	4.18
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	16	4.17
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	5	4.16
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	6	4.15
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	12	3.99
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	12	3.82
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	20	3.74
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	9	3.73
(1,33)	1:26:A:SER:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	7	3.69
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	7	3.65
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	17	3.63
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	8	3.59
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	6	3.52
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	15	3.52
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	14	3.51
(1,32)	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	1:27:A:TYR:N	10	3.44
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	20	3.44
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	7	3.41
(1,10)	1:11:A:TYR:N	1:11:A:TYR:CA	1:11:A:TYR:C	1:12:A:PRO:N	20	3.41
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	3	3.4
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	13	3.37
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	16	3.36
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	4	3.34
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	18	3.32
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	5	3.29
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	18	3.26
(1,33)	1:26:A:SER:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	10	3.24
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	20	3.2
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	5	3.13
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	13	3.11
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	2	3.09
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	8	3.05
(1,33)	1:26:A:SER:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	14	3.03
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	15	3.02
(1,68)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:ASN:N	15	3.01
(1,33)	1:26:A:SER:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	2	2.98
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	17	2.96
(1,30)	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	1:26:A:SER:N	5	2.95
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	18	2.9
(1,33)	1:26:A:SER:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	3	2.88
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	8	2.86
(1,30)	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	1:26:A:SER:N	4	2.8
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	4	2.77
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	5	2.7
(1,33)	1:26:A:SER:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	4	2.67
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	19	2.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	1:27:A:TYR:N	3	2.59
(1,30)	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	1:26:A:SER:N	1	2.57
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	2	2.56
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	10	2.56
(1,9)	1:10:A:PRO:C	1:11:A:TYR:N	1:11:A:TYR:CA	1:11:A:TYR:C	20	2.56
(1,8)	1:10:A:PRO:N	1:10:A:PRO:CA	1:10:A:PRO:C	1:11:A:TYR:N	7	2.53
(1,32)	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	1:27:A:TYR:N	7	2.52
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	17	2.5
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	14	2.48
(1,46)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	2	2.48
(1,28)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:TYR:N	20	2.43
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	18	2.38
(1,32)	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	1:27:A:TYR:N	2	2.35
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	14	2.28
(1,14)	1:15:A:ASN:N	1:15:A:ASN:CA	1:15:A:ASN:C	1:16:A:GLY:N	17	2.24
(1,33)	1:26:A:SER:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	17	2.22
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	13	2.21
(1,80)	1:62:A:TYR:N	1:62:A:TYR:CA	1:62:A:TYR:C	1:63:A:PRO:N	20	2.21
(1,14)	1:15:A:ASN:N	1:15:A:ASN:CA	1:15:A:ASN:C	1:16:A:GLY:N	13	2.2
(1,100)	1:74:A:TYR:N	1:74:A:TYR:CA	1:74:A:TYR:C	1:75:A:GLY:N	11	2.15
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	10	2.14
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	13	2.1
(1,50)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:ASN:N	2	2.06
(1,105)	1:76:A:LYS:C	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	7	2.05
(1,27)	1:23:A:GLY:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	8	2.0
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	6	1.99
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	15	1.95
(1,82)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:TYR:N	20	1.92
(1,28)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:TYR:N	9	1.87
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	19	1.86
(1,50)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:ASN:N	7	1.86
(1,33)	1:26:A:SER:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	5	1.86
(1,105)	1:76:A:LYS:C	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	2	1.85
(1,105)	1:76:A:LYS:C	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	1	1.84
(1,48)	1:37:A:GLY:N	1:37:A:GLY:CA	1:37:A:GLY:C	1:38:A:LYS:N	1	1.83
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	16	1.81
(1,30)	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	1:26:A:SER:N	19	1.8
(1,28)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:TYR:N	16	1.78
(1,105)	1:76:A:LYS:C	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	5	1.75
(1,80)	1:62:A:TYR:N	1:62:A:TYR:CA	1:62:A:TYR:C	1:63:A:PRO:N	14	1.75
(1,14)	1:15:A:ASN:N	1:15:A:ASN:CA	1:15:A:ASN:C	1:16:A:GLY:N	14	1.74
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	4	1.69
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	15	1.68
(1,22)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:LYS:N	15	1.67
(1,38)	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	1:30:A:TYR:N	7	1.66
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	9	1.64
(1,108)	1:78:A:CYS:N	1:78:A:CYS:CA	1:78:A:CYS:C	1:79:A:GLN:N	11	1.61
(1,98)	1:73:A:TYR:N	1:73:A:TYR:CA	1:73:A:TYR:C	1:74:A:TYR:N	15	1.57
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	2	1.57
(1,7)	1:9:A:SER:C	1:10:A:PRO:N	1:10:A:PRO:CA	1:10:A:PRO:C	19	1.57
(1,9)	1:10:A:PRO:C	1:11:A:TYR:N	1:11:A:TYR:CA	1:11:A:TYR:C	7	1.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,105)	1:76:A:LYS:C	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	12	1.55
(1,62)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	1:48:A:ASN:N	11	1.52
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	1	1.52
(1,80)	1:62:A:TYR:N	1:62:A:TYR:CA	1:62:A:TYR:C	1:63:A:PRO:N	12	1.51
(1,28)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:TYR:N	13	1.49
(1,32)	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	1:27:A:TYR:N	14	1.47
(1,8)	1:10:A:PRO:N	1:10:A:PRO:CA	1:10:A:PRO:C	1:11:A:TYR:N	11	1.47
(1,58)	1:45:A:CYS:N	1:45:A:CYS:CA	1:45:A:CYS:C	1:46:A:PHE:N	19	1.46
(1,96)	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	1:72:A:GLY:N	1	1.43
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	13	1.43
(1,40)	1:30:A:TYR:N	1:30:A:TYR:CA	1:30:A:TYR:C	1:31:A:CYS:N	3	1.41
(1,40)	1:30:A:TYR:N	1:30:A:TYR:CA	1:30:A:TYR:C	1:31:A:CYS:N	6	1.4
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	14	1.4
(1,40)	1:30:A:TYR:N	1:30:A:TYR:CA	1:30:A:TYR:C	1:31:A:CYS:N	10	1.38
(1,22)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:LYS:N	19	1.37
(1,103)	1:75:A:GLY:C	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	4	1.36
(1,14)	1:15:A:ASN:N	1:15:A:ASN:CA	1:15:A:ASN:C	1:16:A:GLY:N	6	1.35
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	5	1.33
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	10	1.33
(1,20)	1:19:A:CYS:N	1:19:A:CYS:CA	1:19:A:CYS:C	1:20:A:LYS:N	9	1.32
(1,16)	1:16:A:GLY:N	1:16:A:GLY:CA	1:16:A:GLY:C	1:17:A:GLY:N	12	1.28
(1,3)	1:7:A:PRO:C	1:8:A:CYS:N	1:8:A:CYS:CA	1:8:A:CYS:C	13	1.28
(1,105)	1:76:A:LYS:C	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	19	1.27
(1,45)	1:35:A:TYR:C	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	9	1.26
(1,43)	1:33:A:LYS:C	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	17	1.26
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	12	1.26
(1,20)	1:19:A:CYS:N	1:19:A:CYS:CA	1:19:A:CYS:C	1:20:A:LYS:N	15	1.26
(1,80)	1:62:A:TYR:N	1:62:A:TYR:CA	1:62:A:TYR:C	1:63:A:PRO:N	13	1.25
(1,43)	1:33:A:LYS:C	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	11	1.25
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	8	1.23
(1,14)	1:15:A:ASN:N	1:15:A:ASN:CA	1:15:A:ASN:C	1:16:A:GLY:N	11	1.23
(1,61)	1:46:A:PHE:C	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	11	1.22
(1,43)	1:33:A:LYS:C	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	6	1.22
(1,38)	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	1:30:A:TYR:N	5	1.21
(1,84)	1:65:A:TYR:N	1:65:A:TYR:CA	1:65:A:TYR:C	1:66:A:LYS:N	9	1.2
(1,58)	1:45:A:CYS:N	1:45:A:CYS:CA	1:45:A:CYS:C	1:46:A:PHE:N	8	1.2
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	4	1.2
(1,14)	1:15:A:ASN:N	1:15:A:ASN:CA	1:15:A:ASN:C	1:16:A:GLY:N	10	1.2
(1,32)	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	1:27:A:TYR:N	4	1.17
(1,63)	1:47:A:PRO:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	16	1.15
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	19	1.15
(1,50)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:ASN:N	3	1.14
(1,58)	1:45:A:CYS:N	1:45:A:CYS:CA	1:45:A:CYS:C	1:46:A:PHE:N	2	1.12
(1,43)	1:33:A:LYS:C	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	3	1.12
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	2	1.12
(1,30)	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	1:26:A:SER:N	14	1.1
(1,45)	1:35:A:TYR:C	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	12	1.08
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	18	1.04
(1,68)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:ASN:N	6	1.02
(1,45)	1:35:A:TYR:C	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	19	1.02
(1,29)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	5	1.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,58)	1:45:A:CYS:N	1:45:A:CYS:CA	1:45:A:CYS:C	1:46:A:PHE:N	5	1.01
(1,30)	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	1:26:A:SER:N	11	1.01
(1,103)	1:75:A:GLY:C	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	12	1.0
(1,88)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:SER:N	10	1.0
(1,40)	1:30:A:TYR:N	1:30:A:TYR:CA	1:30:A:TYR:C	1:31:A:CYS:N	19	1.0
(1,33)	1:26:A:SER:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	1	1.0